



Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 07:32 pm BST

PDB ID : 8C8M
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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

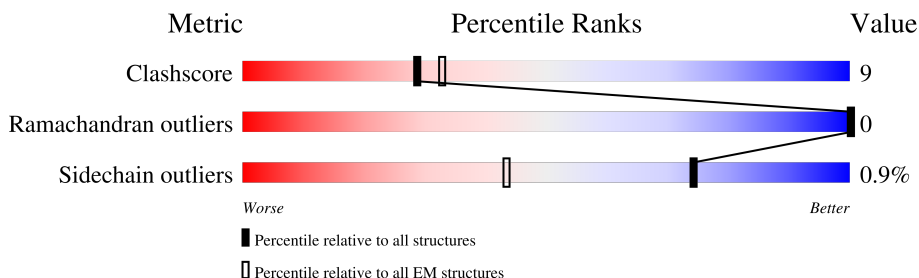
1 Overall quality at a glance

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	
1	E	1734	
1	F	1734	

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		

SER LEU LEU TRP THR GLY SER SER SER GLY GLN SER PHE SER PRO PRO LEU LEU SER SER TRP THR ILE PRO THR PRO GLU ALA ALA GLY THR TYR THR THR THR THR PHE VAL VAL TRP TRP GLU GLY VAL VAL ASP ASN PRO PRO THR THR LEU LEU SER SER PRO PRO VAL SER SER THR THR VAL ASN VAL SER

- Molecule 1: Cell surface protein

Chain B: 73% 18% 9%

[illegible]

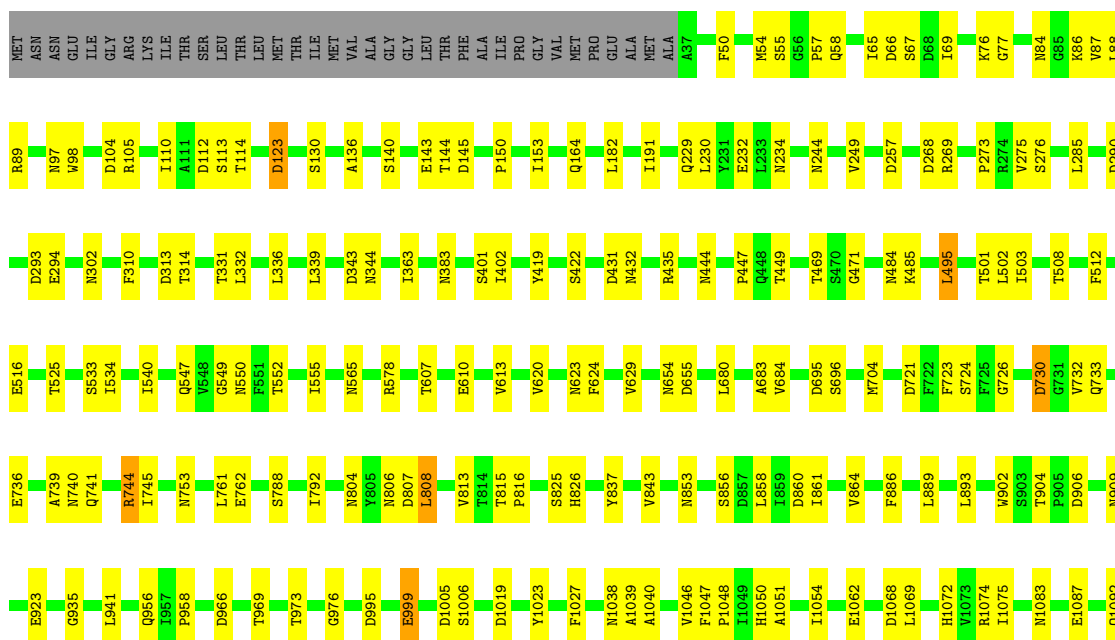
- Molecule 1: Cell surface protein

Chain C:  73% 18% 9%

- Molecule 1: Cell surface protein

Chain D: 73% 18% 9%

D313 T314	L330 T331 L332	L336	L339	D343 N344	Q354	I363	S401 I402	S422	D431 N432	G436	N444	T469 S470 G471 Q472	N484 K485	L495	D499	I500 L502 I503	T508	F512	E516	T525	S633 I534	I540	E547					
W98	Y101	D104 R105	T110 A111	D112 S113 T114 A115	D123	S130	A136	S140	E143 T144 D145	P150	I153	Q164	L182	I191	Q229 L230 Y231	E232	D257	D268 R269	P273 A274 V275 S276	L285	D290	D293 E294	N302					
MET	ASN	GLU	GLY	ARG	LYS	ILE	THR	MET	THR	ILE	MET	VAL	ALA	GLY	LEU	THR	PHE	ALA	ILE	PRO	GLY	VAL	MET	PRO	GLU	ALA	MET	ALA
A37	F42	F50	S55	G56	P57	Q58	E61	I65	D66	S67	D68	I69	V87	L88	R89	N97												



LEU	ASP	TRP	S1641	D1390	E1266	I1098
ILE	SER	ILE	L1550	F1393	I1267	I1098
PRO	SER	PRO	T1551	F1393	Y1268	R1102
GLU	SER	GLU	V1552	E1403	D1269	D1270
ALA	VAL	ALA	T1553	T1404	D1271	S1106
ASP	ASP	GLY	E1554	T1404	E1274	D1122
GLN	GLN	THR	T1555	I1409	W1275	D1122
THR	GLN	TYR	A1558	V1411	D1276	I1133
ALA	GLN	ALA	T1559	V1411	T1281	R1134
THR	ILE	THR	G1560	R1414	S1136	S1136
SER	SER	ALA	F1561	R1414	D1297	F1136
PHE	ALA	PHE	F1562	K1422	P1298	M1139
VAL	ASP	VAL	E1563	L1423	E1299	M1139
TRP	LEU	TRP	G1564	T1423	P1300	T1301
GLU	ALA	GLU	T1565	T1434	T1301	A1143
ASN	ASN	SER	V1566	T1434	R1304	A1146
GLY	GLY	VAL	F1567	I1438	E1305	F1149
ASP	GLN	ASP	S1574	L1439	D1308	S1309
ASN	ASP	PRO	G1575	D1446	S1309	I1315
ARG	ARG	THR	S1576	T1453	E1321	P1161
LEU	GLN	ALA	H1577	P1465	A1162	S1163
THR	SER	PHE	R1578	P1465	A1164	Q1165
SER	SER	SER	L1579	D1473	E1337	L1176
PRO	ALA	PRO	R1580	D1474	D1340	W1341
TYR	LEU	VAL	D1585	V1480	L1201	Q1202
VAL	LEU	VAL	N1594	T1490	G1203	D1204
SER	VAL	SER	T1595	N1499	V1208	P1213
THR	GLN	THR	L1596	I1500	D1230	L1231
VAL	ASP	VAL	P1597	V1503	D1239	K1240
ASN	ALA	VAL	E1605	E1507	E1352	D1353
SER	GLY	VAL	T1616	Y1510	F1365	T1245
THR	THR	THR	VAL	Y1510	Y1376	D1257
VAL	VAL	VAL	VAL	G1516	S1377	W1378
SER	SER	SER	PRO	V1517	T1379	T1379
LEU	SER	SER	ALA	V1520	D1261	N1262
SER	SER	SER	ASN	V1520	D1263	S1264
GLY	GLY	GLY	LEU	Y1376	V1382	I1383
THR	GLN	THR	ARG	D1524	Y1383	I1384
VAL	SER	VAL	THR	P1529	T1385	A1265
PHE	PHE	ASP	ASP	V1532		
ALA	ALA	ALA	ALA			
PRO	PRO	PRO	PRO			
ALA	ALA	ALA	ALA			
LEU	LEU	LEU	LEU			
SER	SER	SER	SER			

● Molecule 1: Cell surface protein

Chain F:  72% 18% 9%

MET	ASN	D104	N302	I534	N740	G935	E1087	L1231
ASN	ASN	R105	F310	I540	R744	A936	Q1092	D1239
GLU	GLU	I110	D313	Q547	I745	T937	I1098	K1240
ILE	ILE	A111	T314	V548	E749	L941	R1102	I1245
ARG	ARG	S113	D314	G549	T750	D954	G1103	D1257
LYS	LYS	T114	N322	N550	G751	P955	S1104	F1258
ILE	ILE	A115	L330	F551	D752	Q956	S1106	
THR	THR	D123	T331	T552	N753	P957	D1122	D1261
LEU	LEU	S130	L332	I555	L761	D966		N1262
THR	THR	A136	R333	N555	E762	T969	I1133	D1263
LEU	LEU	I153	T334	R578	S788	T973	R1134	A1265
MET	MET	Q164	T335	I580	I792	T973	S1135	I1267
ILE	ILE	L182	D343	L579	T804	G976	F1136	Y1268
THR	THR	I191	N344	I580	T805		M1139	D1269
GLN	GLN	A197	T363	T607	N806	G983	A1143	L1270
ASP	ASP	P226	S401	E610	L808	L984	A1146	E1274
ALA	ALA	I153	I402	V613	V813	D985		W1275
GLY	GLY	Q164	P411	V620	T814	D995	D1152	D1276
THR	THR	L182	Y419	N623	T815	E999	V1153	T1281
LEU	LEU	I191	E421	V629	P816	D1005	N1154	D1297
PRO	PRO	A197	S422	N654	S825	S1006	P1161	P1298
GLU	GLU	A197	D431	D655	H826	D1019	A1162	E1299
ASP	ASP	P226	N432	L680	Y837	Y1023	A1164	P1300
ALA	ALA	Q229	R435	L680	V843	F1027	Q1165	T1301
GLY	GLY	L230	G436	A683	N853	N1038	L1176	D1308
THR	THR	E232	N444	V684	L858	A1039	L1201	S1309
SER	SER	F42	T469	D695	I859	V1046	Q1202	I1315
LEU	LEU	F50	Q472	S696	D860	F1047	G1203	E1321
ALA	ALA	Q58	D268	M704	V864	P1048	D1204	S1322
SER	SER	T65	R269	V717	F886	H1050	I1205	K1327
GLY	GLY	S67	P273	D721	L889	A1051	Q1207	R1330
LEU	LEU	D68	V275	D721	L893	I1054	V1208	E1337
SER	SER	D68	S276	S724	L893	E1062	P1213	D1340
SER	SER	L69	L502	F725	W902		S1217	W1341
GLY	GLY	V67	L503	G726	S903	D1068	G1218	D1345
THR	THR	L88	F512	D730	T904	L1069	D1219	S1346
ASP	ASP	R89	E516	G731	P905	H1072	N1221	D1347
ALA	ALA	Y94	D290	V732	D906	H1072	T1222	Y1348
PRO	PRO	N97	D293	Q733	N909	I1075	T1224	V1349
ALA	ALA	Y98	E294	E736	E923	M1083	D1225	E1352
SER	SER		S533	A739			S1226	D1353
							D1230	

ASN	V1369	
LEU		
SER	D1372	
GLY		
ARG	Y1376	
THR	S1377	
VAL	Y1378	
ASP	T1379	
ALA		
PHE	V1382	
PRO	Y1383	
ASN	I1384	
LEU	T1385	
TRP		
ILE	S1541	
ASP		
SER	F1393	
THR		
VAL	L1550	
GLU	T1551	
ALA	V1552	
GLY	T1553	
THR	E1554	
TYR	T1555	
THR		
VAL		
ALA	I1409	
GLN	K1410	
THR	T1559	
ILE	V1411	
THR		
ALA	R1414	
PHE		
ASP	I1561	
ASN	F1562	
PRO	E1563	
THR	G1564	
LEU	T1565	
GLY	V1566	
VAL	F1567	
ASP		
ASN	S1574	
PRO		
THR	L1578	
GLU	I1579	
ALA	R1580	
GLN		
SER	D1446	
LEU		
THR	T1453	
PRO		
VAL	P1465	
THR		
SER	L1469	
THR		
ILE	T1595	
GLN	L1596	
VAL	P1597	
ASN		
VAL	E1605	
SER		
	T1618	
THR	VAL	
VAL	VAL	
SER	PRO	
LEU	PRO	
ALA	LEU	
ALA	TRP	
ILE	ILE	
THR	THR	
GLY	GLY	
SER	PRO	
LEU	ALA	

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 (\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 (\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	0.75	9/11941 (0.1%)	0.81	18/16339 (0.1%)
1	B	0.69	2/11941 (0.0%)	0.77	8/16339 (0.0%)
1	C	0.69	2/11941 (0.0%)	0.77	6/16339 (0.0%)
1	D	0.68	1/11941 (0.0%)	0.76	7/16339 (0.0%)
1	E	0.69	2/11941 (0.0%)	0.77	7/16339 (0.0%)
1	F	0.70	3/11941 (0.0%)	0.77	5/16339 (0.0%)
All	All	0.70	19/71646 (0.0%)	0.77	51/98034 (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 (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	793	GLU	CD-OE2	16.03	1.43	1.25
1	A	1255	GLU	CD-OE1	-15.38	1.08	1.25
1	A	793	GLU	CD-OE1	-13.35	1.10	1.25
1	A	196	GLU	CD-OE1	-10.86	1.13	1.25
1	A	1299	GLU	CD-OE1	-9.95	1.14	1.25
1	F	858	LEU	C-O	-8.47	1.07	1.23
1	C	858	LEU	C-O	-8.44	1.07	1.23
1	D	858	LEU	C-O	-7.86	1.08	1.23
1	A	858	LEU	C-O	-7.75	1.08	1.23
1	B	858	LEU	C-O	-7.45	1.09	1.23
1	E	858	LEU	C-O	-7.41	1.09	1.23
1	C	808	LEU	C-O	-5.62	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	808	LEU	C-O	-5.55	1.12	1.23
1	F	1399	ASP	CG-OD1	-5.41	1.12	1.25
1	A	1329	GLU	CD-OE2	-5.38	1.19	1.25
1	A	1425	GLU	CD-OE1	5.15	1.31	1.25
1	E	808	LEU	C-O	-5.12	1.13	1.23
1	B	808	LEU	C-O	-5.07	1.13	1.23
1	A	1299	GLU	CD-OE2	-5.04	1.20	1.25

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	729	ASP	CB-CG-OD1	15.40	132.16	118.30
1	A	123	ASP	CB-CG-OD1	11.60	128.74	118.30
1	A	794	ASP	CB-CG-OD2	10.58	127.82	118.30
1	A	729	ASP	CB-CG-OD2	-9.00	110.20	118.30
1	E	1257	ASP	CB-CG-OD1	-8.15	110.96	118.30
1	A	793	GLU	CG-CD-OE2	8.12	134.55	118.30
1	B	1257	ASP	CB-CG-OD1	-8.12	110.99	118.30
1	A	729	ASP	CA-CB-CG	7.90	130.77	113.40
1	D	1257	ASP	CB-CG-OD1	-7.82	111.27	118.30
1	F	1257	ASP	CB-CG-OD1	-7.71	111.36	118.30
1	A	794	ASP	CB-CG-OD1	-7.66	111.41	118.30
1	D	58	GLN	CB-CA-C	-7.20	96.00	110.40
1	A	58	GLN	CB-CA-C	-7.18	96.03	110.40
1	C	58	GLN	CB-CA-C	-7.10	96.20	110.40
1	F	38	ASN	CB-CA-C	6.91	124.22	110.40
1	B	58	GLN	CB-CA-C	-6.70	97.01	110.40
1	E	58	GLN	CB-CA-C	-6.31	97.78	110.40
1	A	793	GLU	CG-CD-OE1	-6.26	105.78	118.30
1	D	1340	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	A	1299	GLU	OE1-CD-OE2	-6.20	115.86	123.30
1	A	1255	GLU	OE1-CD-OE2	-6.10	115.98	123.30
1	C	1257	ASP	CB-CG-OD1	-6.05	112.86	118.30
1	E	1340	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	B	1340	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	A	1257	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	730	ASP	CB-CG-OD2	5.86	123.58	118.30
1	B	744	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	C	1340	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	A	729	ASP	OD1-CG-OD2	-5.75	112.38	123.30
1	F	1340	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	E	744	ARG	NE-CZ-NH1	5.68	123.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	510	ASP	CB-CG-OD2	5.54	123.28	118.30
1	B	1578	ARG	CG-CD-NE	-5.37	100.52	111.80
1	B	730	ASP	CB-CG-OD2	5.30	123.07	118.30
1	C	550	ASN	CB-CA-C	5.21	120.83	110.40
1	D	1578	ARG	CG-CD-NE	-5.21	100.85	111.80
1	F	550	ASN	CB-CA-C	5.21	120.82	110.40
1	A	1578	ARG	CG-CD-NE	-5.19	100.89	111.80
1	E	730	ASP	CB-CG-OD2	5.18	122.97	118.30
1	D	550	ASN	CB-CA-C	5.17	120.73	110.40
1	A	550	ASN	CB-CA-C	5.16	120.71	110.40
1	A	744	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	B	550	ASN	CB-CA-C	5.11	120.62	110.40
1	E	123	ASP	CB-CG-OD1	5.11	122.89	118.30
1	E	550	ASN	CB-CA-C	5.10	120.60	110.40
1	D	744	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	D	730	ASP	CB-CG-OD2	5.07	122.86	118.30
1	C	123	ASP	CB-CG-OD1	5.05	122.85	118.30
1	F	123	ASP	CB-CG-OD1	5.03	122.83	118.30
1	C	730	ASP	CB-CG-OD2	5.01	122.81	118.30
1	B	123	ASP	CB-CG-OD1	5.01	122.81	118.30

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	245	0
1	B	11751	0	10951	221	0
1	C	11751	0	10951	248	0
1	D	11751	0	10951	252	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	11751	0	10949	221	0
1	F	11751	0	10951	248	0
All	All	70506	0	65704	1252	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 9.

All (1252) 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
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: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:C:985:ASP:OD1	1:D:1394:ASP:OD2	1.85	0.94
1:A:1329:GLU:OE1	1:A:1486:GLU:CD	2.06	0.93
1:B:1567:PHE:HD2	1:B:1578:ARG:HG3	1.32	0.93
1:A:1394:ASP:OD2	1:F:985:ASP:OD1	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:E:275:VAL:O	1:E:275:VAL:HG12	1.97	0.63
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: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:B:86:LYS:HG2	1:C:322:ASN:HB2	1.80	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: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
1:A:1455:ASP:OD1	1:F:1104:SER:CB	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1098:ILE:HG13	1:F:1208:VAL:HG12	1.88	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:1321:GLU:CD	1:D:1393:PHE:CD1	2.82	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
1:D:1321:GLU:CD	1:D:1393:PHE:CG	2.81	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:739:ALA:HB2	1:B:792:ILE:HG13	1.91	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: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: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:322:ASN:OD1	1:C:322:ASN:C	2.48	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:F:322:ASN:C	1:F:322:ASN:OD1	2.48	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:813:VAL:HG11	1:F:956:GLN:CD	2.33	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
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: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:B:813:VAL:HG11	1:C:956:GLN:CD	2.33	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:B:1075:ILE:HD12	1:B:1139:MET:CE	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:1075:ILE:HD12	1:E:1139:MET:CE	2.43	0.48
1:F:110:ILE:O	1:F:113:SER:OG	2.31	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: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
1:F:1559:THR:HG23	1:F:1561:ILE:H	1.78	0.48
1:A:629:VAL:HG11	1:A:704:MET:HE3	1.96	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:1269:ASP:CG	1:D:1271:ASP:OD2	2.52	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:A:1269:ASP:CG	1:A:1271:ASP:OD2	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:1269:ASP:CG	1:E:1271:ASP:OD2	2.52	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: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:C:1269:ASP:CG	1:C:1271:ASP:OD2	2.52	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: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
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:1075:ILE:HD12	1:A:1139:MET:HE3	1.96	0.47
1:A:1239:ASP:OD1	1:A:1240:LYS:N	2.46	0.47
1:A:1534:ASN:CG	1:F:1205:ILE:HG12	2.34	0.47
1:B:1269:ASP:CG	1:B:1271:ASP:OD2	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:629:VAL:HG11	1:C:704:MET:HE3	1.97	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:D:1075:ILE:HD12	1:D:1139:MET:CE	2.45	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:C:1205:ILE:HG12	1:D:1534:ASN:CG	2.34	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1258:PHE:HB3	1:D:1268:TYR:CE2	2.50	0.47
1:E:886:PHE:C	1:F:1301:THR:HG21	2.36	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:F:1269:ASP:CG	1:F:1271:ASP:OD2	2.53	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: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:956:GLN:CD	1:F:813:VAL:HG11	2.35	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
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:F:1075:ILE:HD12	1:F:1139:MET:CE	2.45	0.46
1:A:1075:ILE:HD12	1:A:1139:MET:CE	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1075:ILE:HD12	1:C:1139:MET:CE	2.45	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: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:C:1075:ILE:HD12	1:C:1139:MET:HE3	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:1027:PHE:HB3	1:F:1349:VAL:HB	1.98	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
1:E:1596:LEU:HD12	1:E:1597:PRO:CD	2.44	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:629:VAL:HG11	1:F:704:MET:HE3	1.98	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: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: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
1:E:525:THR:HG21	1:E:555:ILE:CD1	2.46	0.45
1:A:739:ALA:HB2	1:A:792:ILE:HG12	1.98	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:739:ALA:HB2	1:F:792:ILE:HG12	1.98	0.45
1:C:813:VAL:HG11	1:D:956:GLN:CD	2.37	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:B:1075:ILE:HD12	1:B:1139:MET:HE3	1.99	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:D:629:VAL:HG11	1:D:704:MET:HE3	1.99	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:D:1075:ILE:HD12	1:D:1139:MET:HE3	1.99	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: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: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: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:C:1005:ASP:OD2	1:C:1006:SER:N	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:886:PHE:C	1:C:1301:THR:HG21	2.37	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:1321:GLU:OE1	1:C:1393:PHE:CE1	2.71	0.44
1:A:1465:PRO:CD	1:F:1219:ASP:CB	2.96	0.43
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:629:VAL:HG11	1:A:704:MET:CE	2.49	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: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:1352:GLU:CD	1:B:1578:ARG:CZ	2.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:629:VAL:HG11	1:F:704:MET:CE	2.48	0.43
1:F:1541:SER:OG	1:F:1585:ASP:OD1	2.37	0.43
1:A:813:VAL:HG11	1:B:956:GLN:CD	2.39	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
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: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:D:813:VAL:HG11	1:E:956:GLN:CD	2.39	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: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:1541:SER:OG	1:E:1585:ASP:OD1	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:629:VAL:HG11	1:D:704:MET:CE	2.49	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:E:431:ASP:OD1	1:E:432:ASN:N	2.52	0.42
1:E:629:VAL:HG11	1:E:704:MET:CE	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:629:VAL:HG11	1:E:704:MET:HE3	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
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:629:VAL:HG11	1:B:704:MET:HE3	2.02	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: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:B:153:ILE:HD13	1:B:164:GLN:HB2	2.02	0.42
1:B:629:VAL:HG11	1:B:704:MET:CE	2.49	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:344:ASN:HB3	1:D:444:ASN:OD1	2.20	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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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:1075:ILE:HD12	1:E:1139:MET:HE1	2.03	0.41
1:E:1321:GLU:OE1	1:E:1393:PHE:CE1	2.72	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:65:ILE:HG12	1:B:97:ASN:CG	2.41	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:853:ASN:HA	1:E:860:ASP:OD2	2.20	0.41
1:F:65:ILE:HG12	1:F:97:ASN:CG	2.41	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:65:ILE:HG12	1:A:97:ASN:CG	2.41	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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:65:ILE:HG12	1:D:97:ASN:CG	2.41	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:1529:PRO:O	1:D:1558:ALA:HB2	2.21	0.40
1:E:65:ILE:HG12	1:E:97:ASN:CG	2.41	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: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%)	1300 (99%)	12 (1%)	75	91
1	B	1312/1438 (91%)	1301 (99%)	11 (1%)	79	92
1	C	1312/1438 (91%)	1302 (99%)	10 (1%)	79	92
1	D	1312/1438 (91%)	1300 (99%)	12 (1%)	75	91
1	E	1312/1438 (91%)	1300 (99%)	12 (1%)	75	91
1	F	1312/1438 (91%)	1300 (99%)	12 (1%)	75	91
All	All	7872/8628 (91%)	7803 (99%)	69 (1%)	74	91

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	269	ARG
1	A	419	TYR
1	A	422	SER

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Mol	Chain	Res	Type
1	A	495	LEU
1	A	499	ASP
1	A	565	ASN
1	A	578	ARG
1	A	1047	PHE
1	A	1330	ARG
1	A	1378	TRP
1	A	1414	ARG
1	A	1575	SER
1	B	269	ARG
1	B	419	TYR
1	B	422	SER
1	B	495	LEU
1	B	501	THR
1	B	565	ASN
1	B	578	ARG
1	B	1047	PHE
1	B	1330	ARG
1	B	1378	TRP
1	B	1414	ARG
1	C	269	ARG
1	C	274	ARG
1	C	419	TYR
1	C	495	LEU
1	C	565	ASN
1	C	578	ARG
1	C	1047	PHE
1	C	1330	ARG
1	C	1378	TRP
1	C	1414	ARG
1	D	269	ARG
1	D	422	SER
1	D	495	LEU
1	D	499	ASP
1	D	501	THR
1	D	565	ASN
1	D	578	ARG
1	D	1047	PHE
1	D	1330	ARG
1	D	1378	TRP
1	D	1414	ARG
1	D	1575	SER

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Mol	Chain	Res	Type
1	E	269	ARG
1	E	419	TYR
1	E	422	SER
1	E	495	LEU
1	E	501	THR
1	E	565	ASN
1	E	578	ARG
1	E	999	GLU
1	E	1047	PHE
1	E	1330	ARG
1	E	1378	TRP
1	E	1414	ARG
1	F	38	ASN
1	F	58	GLN
1	F	269	ARG
1	F	274	ARG
1	F	419	TYR
1	F	495	LEU
1	F	565	ASN
1	F	578	ARG
1	F	1047	PHE
1	F	1330	ARG
1	F	1378	TRP
1	F	1414	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	92	GLN
1	A	97	ASN
1	A	211	GLN
1	A	623	ASN
1	A	682	ASN
1	A	733	GLN
1	A	740	ASN
1	A	804	ASN
1	A	956	GLN
1	A	1154	ASN
1	B	58	GLN
1	B	84	ASN
1	B	92	GLN

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Mol	Chain	Res	Type
1	B	97	ASN
1	B	211	GLN
1	B	484	ASN
1	B	623	ASN
1	B	733	GLN
1	B	740	ASN
1	B	804	ASN
1	B	853	ASN
1	B	956	GLN
1	B	1083	ASN
1	B	1154	ASN
1	C	58	GLN
1	C	92	GLN
1	C	97	ASN
1	C	211	GLN
1	C	484	ASN
1	C	623	ASN
1	C	733	GLN
1	C	740	ASN
1	C	804	ASN
1	C	956	GLN
1	C	1083	ASN
1	C	1154	ASN
1	C	1577	HIS
1	D	58	GLN
1	D	92	GLN
1	D	97	ASN
1	D	211	GLN
1	D	623	ASN
1	D	733	GLN
1	D	740	ASN
1	D	804	ASN
1	D	956	GLN
1	D	1083	ASN
1	D	1154	ASN
1	E	58	GLN
1	E	84	ASN
1	E	92	GLN
1	E	97	ASN
1	E	211	GLN
1	E	484	ASN
1	E	623	ASN

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Mol	Chain	Res	Type
1	E	733	GLN
1	E	740	ASN
1	E	804	ASN
1	E	853	ASN
1	E	956	GLN
1	E	1083	ASN
1	E	1154	ASN
1	F	58	GLN
1	F	92	GLN
1	F	97	ASN
1	F	211	GLN
1	F	623	ASN
1	F	733	GLN
1	F	740	ASN
1	F	804	ASN
1	F	956	GLN
1	F	1083	ASN
1	F	1154	ASN
1	F	1577	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.

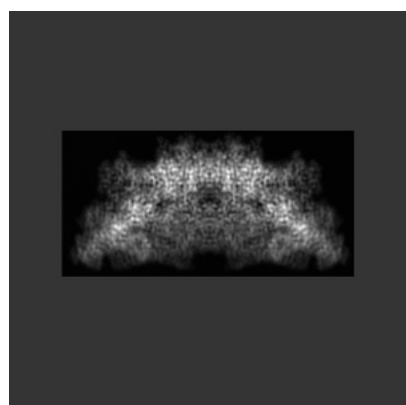
6 Map visualisation [i](#)

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

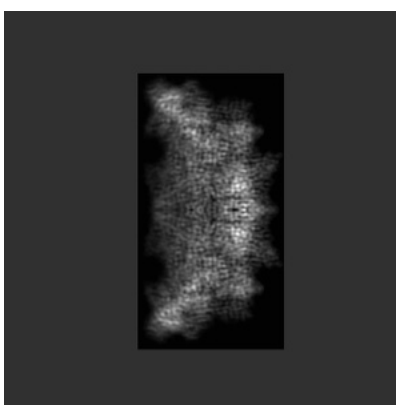
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

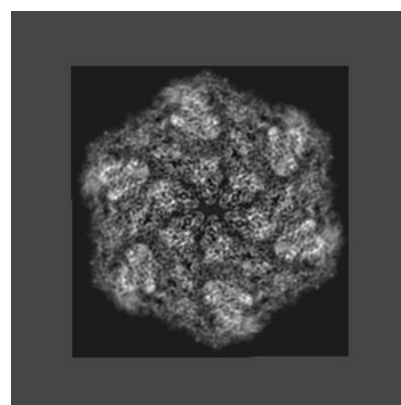
6.1.1 Primary map



X



Y

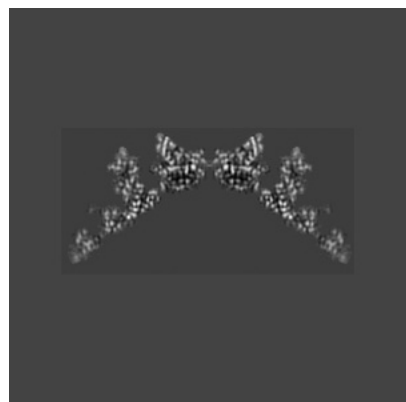


Z

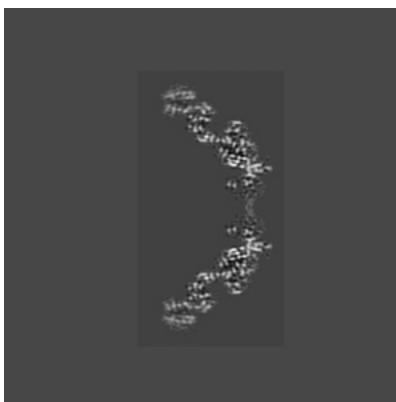
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 160



Y Index: 160



Z Index: 160

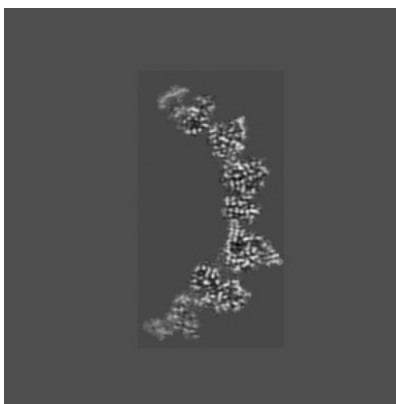
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 156



Y Index: 175

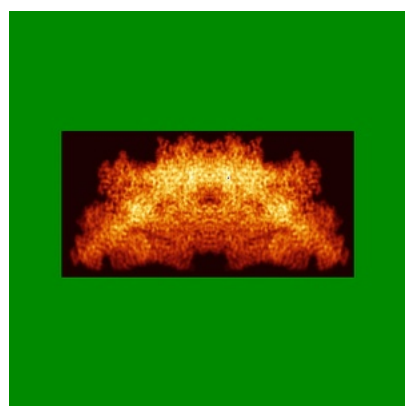


Z Index: 186

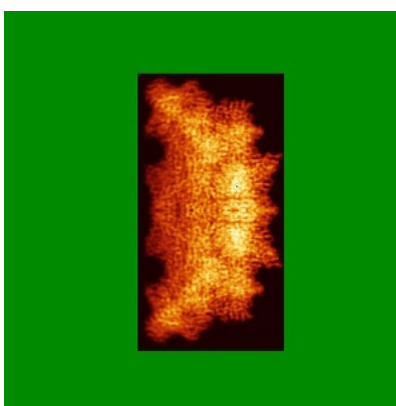
The images above show the largest variance slices of the map in three orthogonal directions.

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

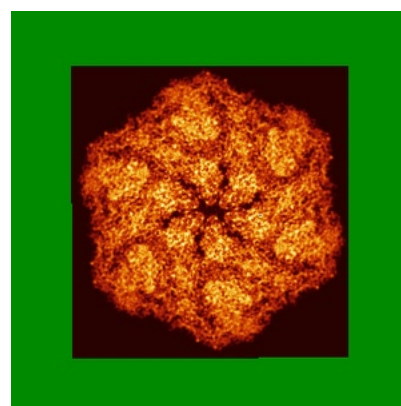
6.4.1 Primary map



X



Y

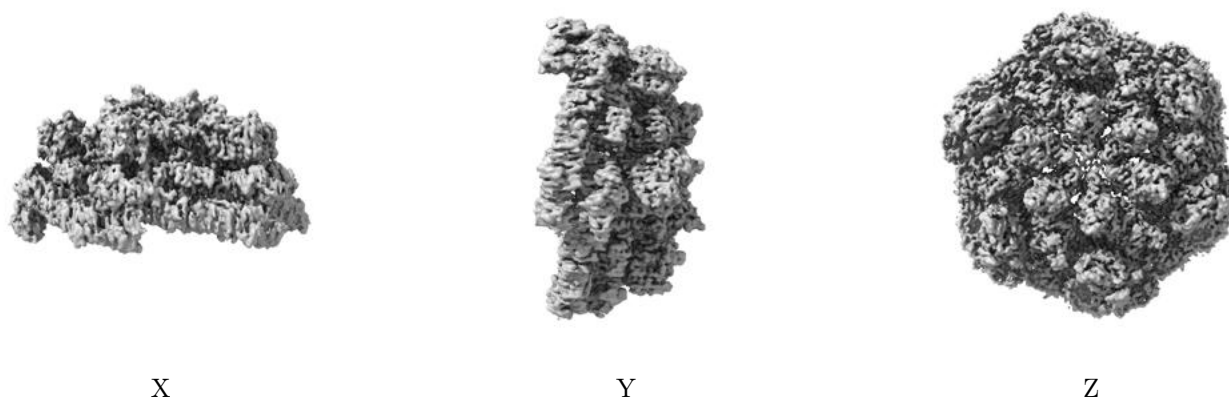


Z

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.

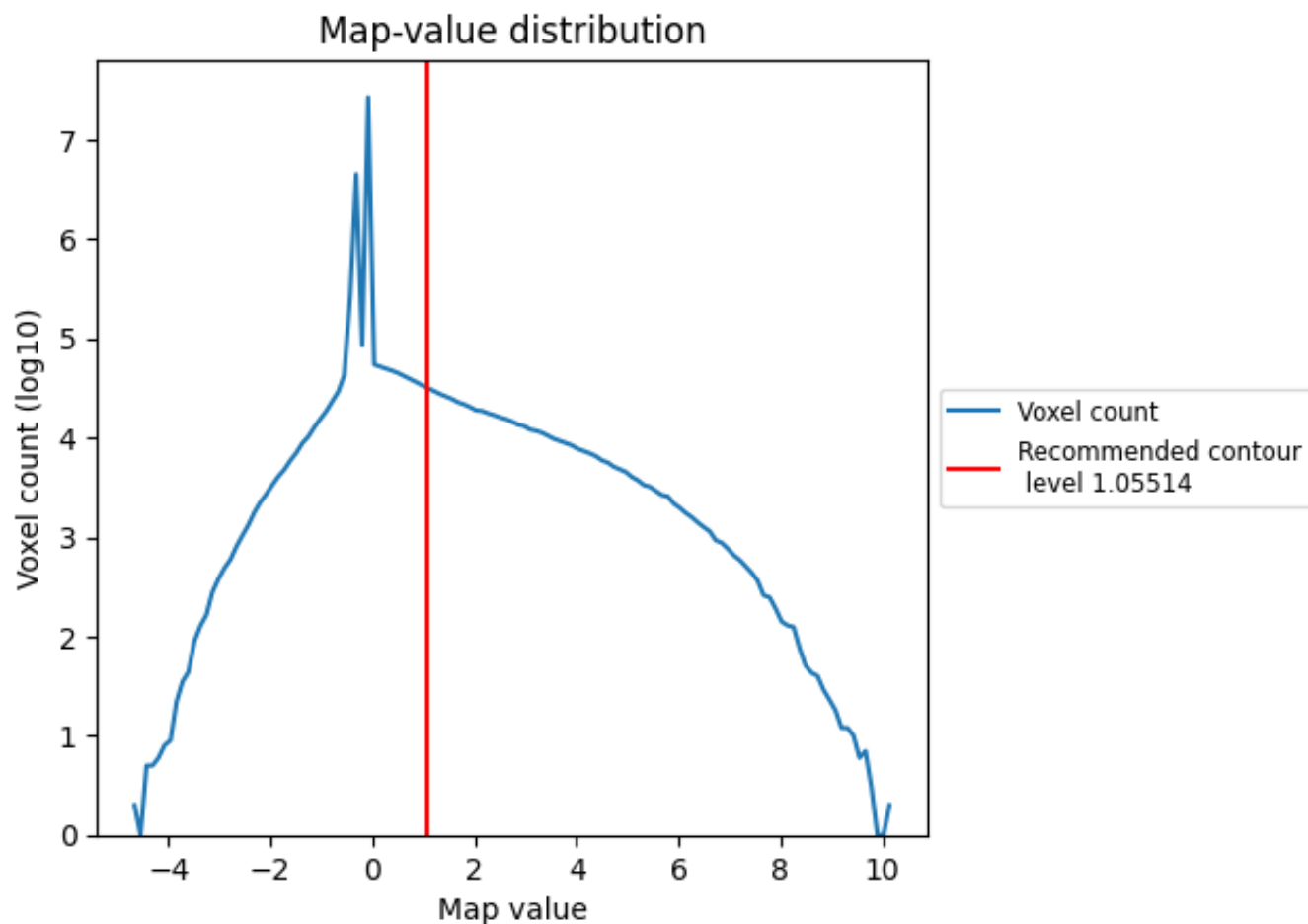
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

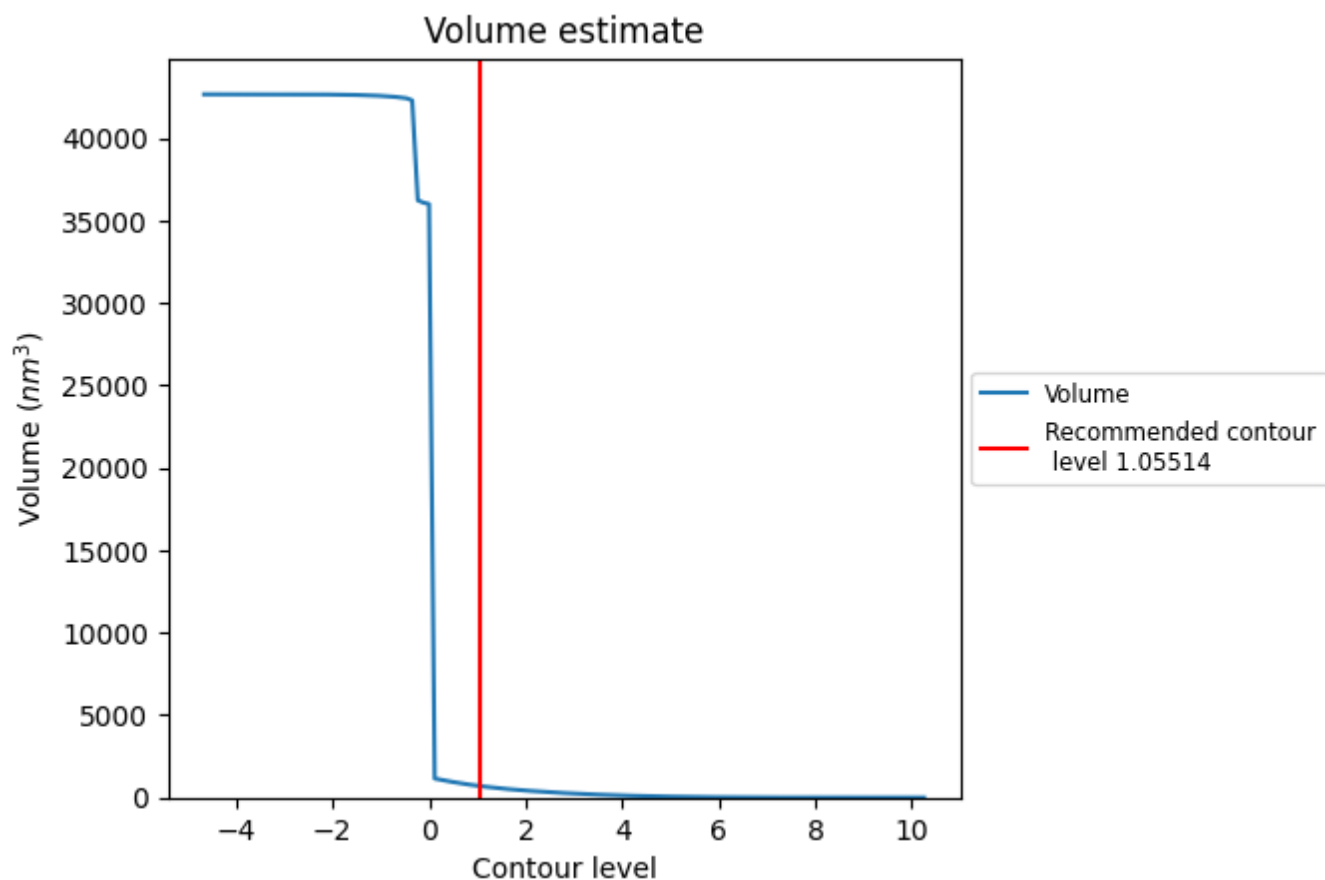
This section contains the results of statistical analysis of the map.

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.

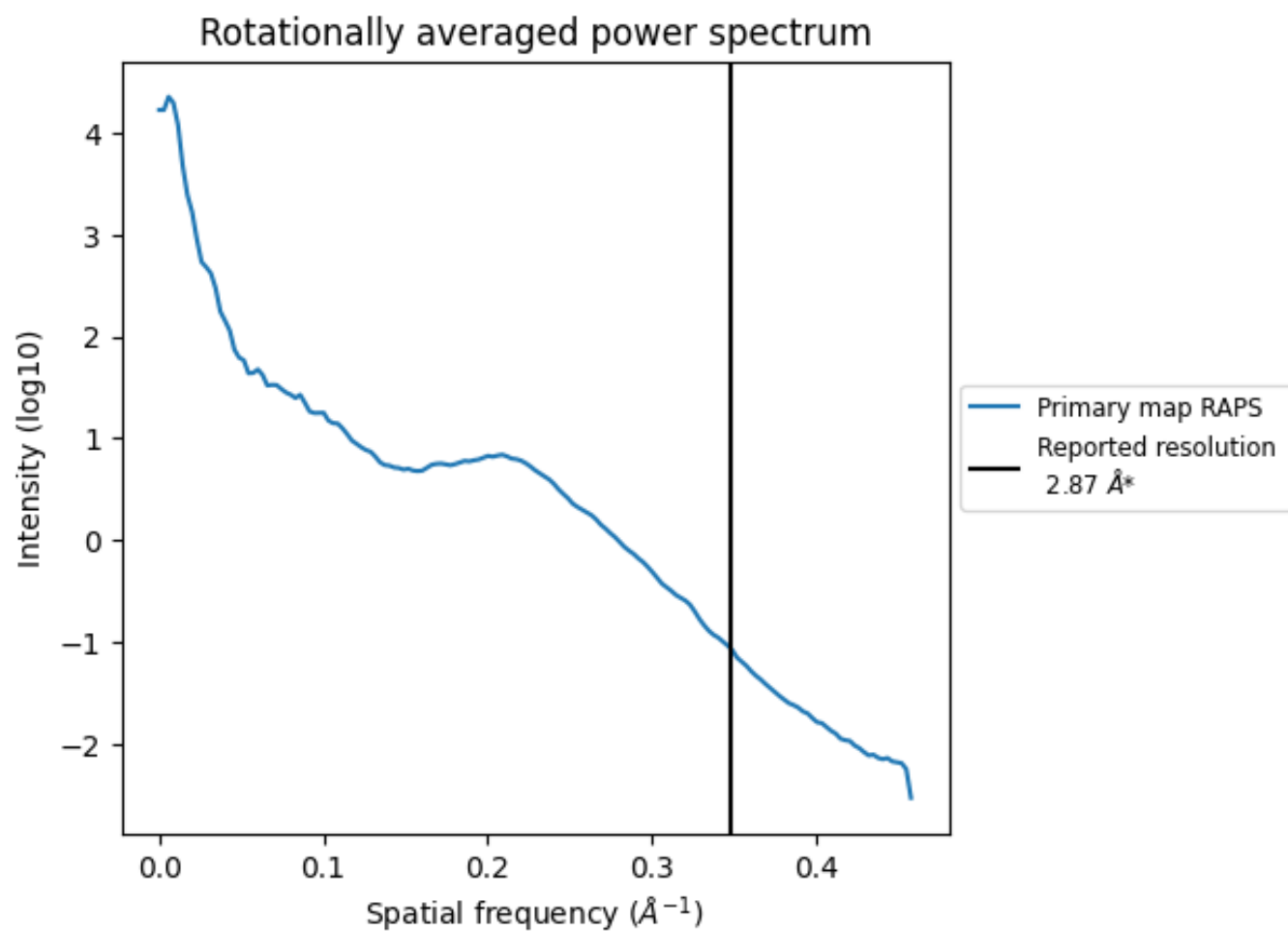
7.2 Volume estimate [i](#)



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 \AA^{-1}

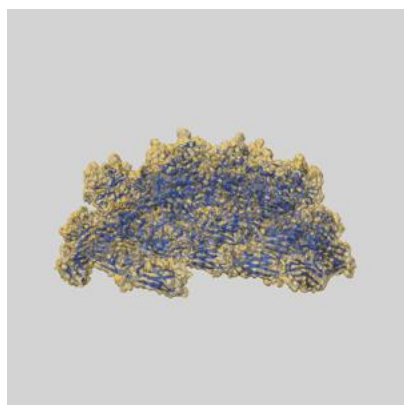
8 Fourier-Shell correlation

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

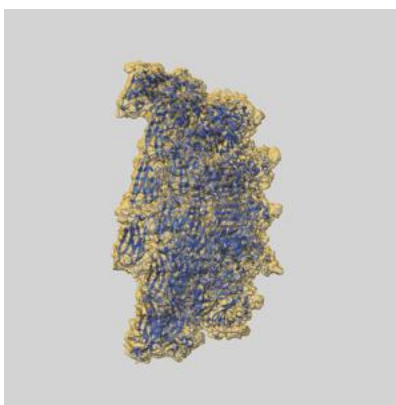
9 Map-model fit [i](#)

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 4](#).

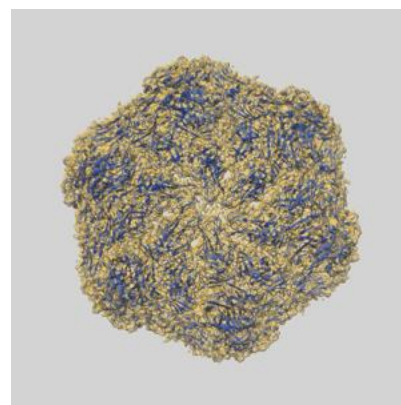
9.1 Map-model overlay [i](#)



X



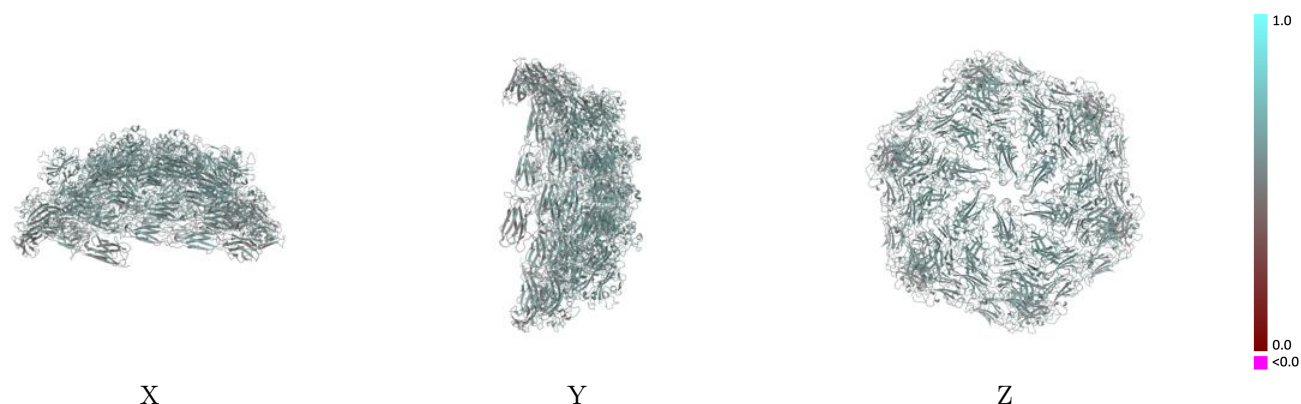
Y



Z

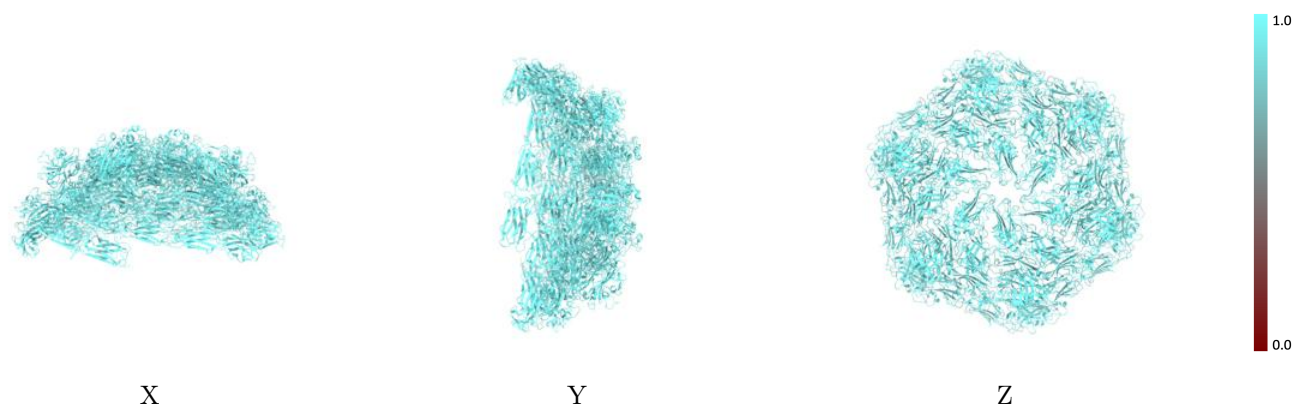
The images above show the 3D surface view of the map at the recommended contour level 1.05514 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



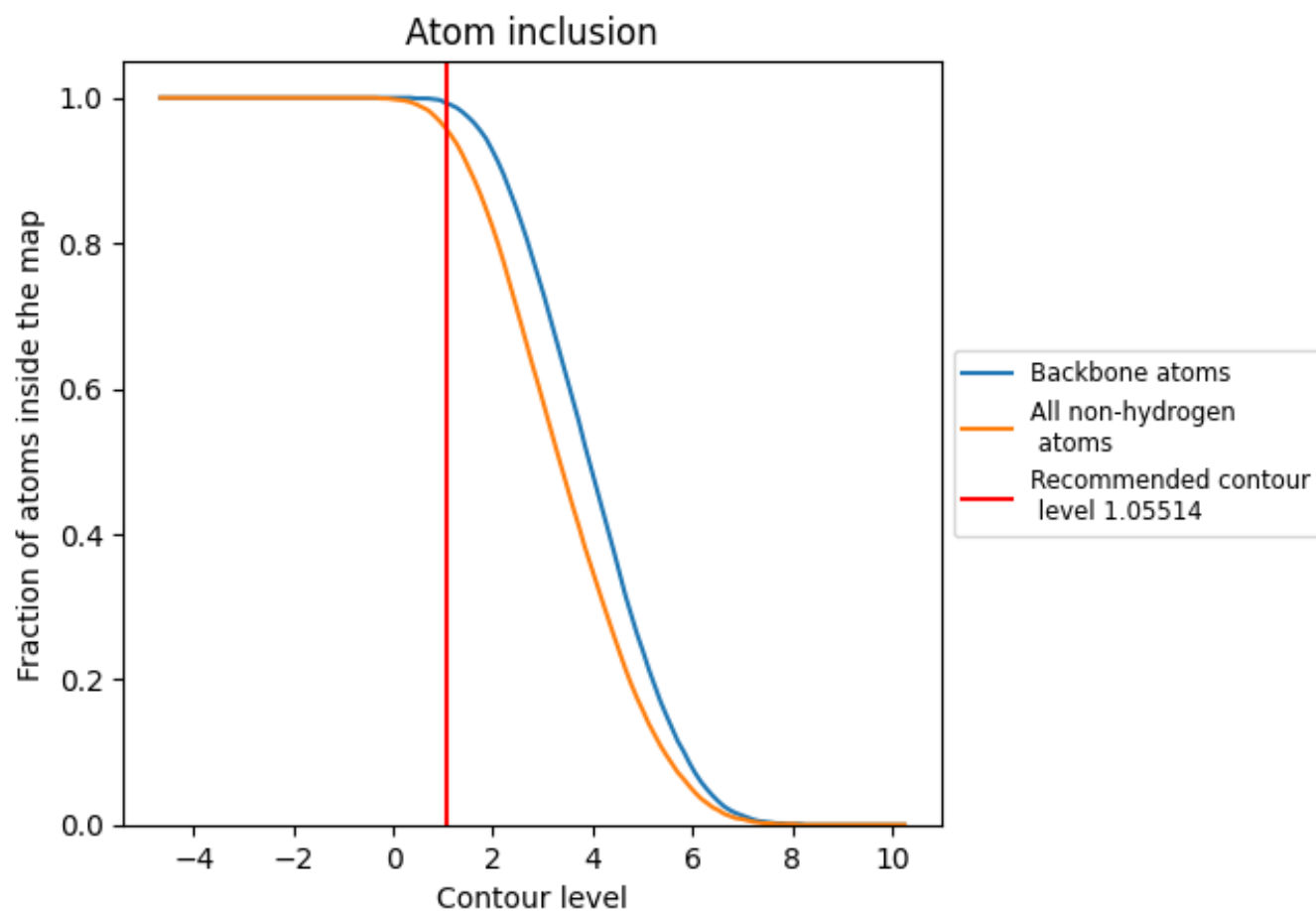
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	<div><div></div></div> 0.9580	<div><div></div></div> 0.5560
A	<div><div></div></div> 0.9620	<div><div></div></div> 0.5630
B	<div><div></div></div> 0.9580	<div><div></div></div> 0.5530
C	<div><div></div></div> 0.9530	<div><div></div></div> 0.5520
D	<div><div></div></div> 0.9630	<div><div></div></div> 0.5620
E	<div><div></div></div> 0.9580	<div><div></div></div> 0.5530
F	<div><div></div></div> 0.9540	<div><div></div></div> 0.5520

1.0

0.0

<0.0