



Full wwPDB EM Validation Report ⓘ

Apr 9, 2026 – 01:38 AM UTC

PDB ID : 9VED / pdb_00009ved
EMDB ID : EMD-64998
Title : The cryo-EM structure of mouse Piezo1-MDFI complex
Authors : Zhang, Y.; Dai, F.
Deposited on : 2025-06-09
Resolution : 3.63 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

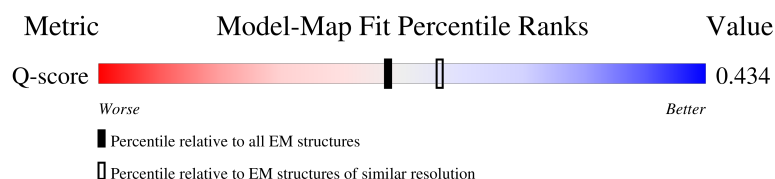
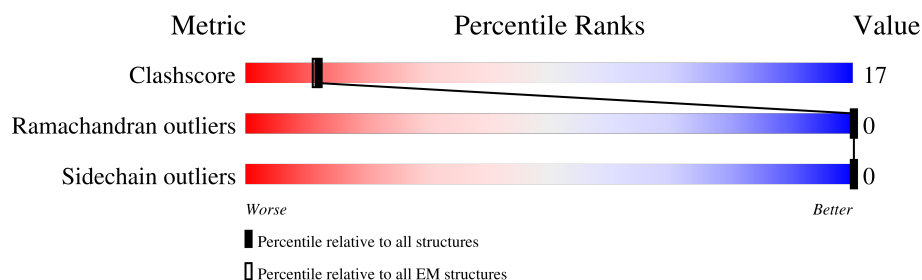
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.63 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.



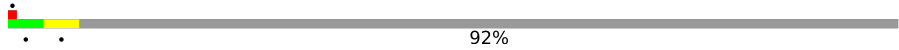

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11696 (3.13 - 4.13)

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	2815	 5% 29% 14% 57%
1	B	2815	 5% 29% 14% 57%
1	C	2815	 5% 29% 14% 57%
2	D	269	 6% 92%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	269	 92%
2	F	269	 92%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29400 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 Piezo-type mechanosensitive ion channel component 1, Green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1223	Total	C	N	O	S	0	0
			9652	6324	1626	1651	51		
1	C	1223	Total	C	N	O	S	0	0
			9652	6324	1626	1651	51		
1	B	1223	Total	C	N	O	S	0	0
			9652	6324	1626	1651	51		

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2548	SER	-	linker	UNP E2JF22
A	2549	ASN	-	linker	UNP E2JF22
A	2550	SER	-	linker	UNP E2JF22
A	2551	LEU	-	linker	UNP E2JF22
A	2552	GLU	-	linker	UNP E2JF22
A	2553	VAL	-	linker	UNP E2JF22
A	2554	LEU	-	linker	UNP E2JF22
A	2555	PHE	-	linker	UNP E2JF22
A	2556	GLN	-	linker	UNP E2JF22
A	2557	GLY	-	linker	UNP E2JF22
A	2558	PRO	-	linker	UNP E2JF22
A	2559	THR	-	linker	UNP E2JF22
A	2560	ALA	-	linker	UNP E2JF22
A	2561	ALA	-	linker	UNP E2JF22
A	2562	ALA	-	linker	UNP E2JF22
A	2563	ALA	-	linker	UNP E2JF22
A	2564	VAL	-	linker	UNP E2JF22
A	2627	LEU	PHE	conflict	UNP P42212
A	2628	THR	SER	conflict	UNP P42212
A	2769	LYS	ALA	conflict	UNP P42212
A	2794	LEU	HIS	conflict	UNP P42212
A	2802	SER	-	expression tag	UNP P42212
A	2803	GLY	-	expression tag	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	2804	GLY	-	expression tag	UNP P42212
A	2805	GLY	-	expression tag	UNP P42212
A	2806	HIS	-	expression tag	UNP P42212
A	2807	HIS	-	expression tag	UNP P42212
A	2808	HIS	-	expression tag	UNP P42212
A	2809	HIS	-	expression tag	UNP P42212
A	2810	HIS	-	expression tag	UNP P42212
A	2811	HIS	-	expression tag	UNP P42212
A	2812	HIS	-	expression tag	UNP P42212
A	2813	HIS	-	expression tag	UNP P42212
A	2814	HIS	-	expression tag	UNP P42212
A	2815	HIS	-	expression tag	UNP P42212
C	2548	SER	-	linker	UNP E2JF22
C	2549	ASN	-	linker	UNP E2JF22
C	2550	SER	-	linker	UNP E2JF22
C	2551	LEU	-	linker	UNP E2JF22
C	2552	GLU	-	linker	UNP E2JF22
C	2553	VAL	-	linker	UNP E2JF22
C	2554	LEU	-	linker	UNP E2JF22
C	2555	PHE	-	linker	UNP E2JF22
C	2556	GLN	-	linker	UNP E2JF22
C	2557	GLY	-	linker	UNP E2JF22
C	2558	PRO	-	linker	UNP E2JF22
C	2559	THR	-	linker	UNP E2JF22
C	2560	ALA	-	linker	UNP E2JF22
C	2561	ALA	-	linker	UNP E2JF22
C	2562	ALA	-	linker	UNP E2JF22
C	2563	ALA	-	linker	UNP E2JF22
C	2564	VAL	-	linker	UNP E2JF22
C	2627	LEU	PHE	conflict	UNP P42212
C	2628	THR	SER	conflict	UNP P42212
C	2769	LYS	ALA	conflict	UNP P42212
C	2794	LEU	HIS	conflict	UNP P42212
C	2802	SER	-	expression tag	UNP P42212
C	2803	GLY	-	expression tag	UNP P42212
C	2804	GLY	-	expression tag	UNP P42212
C	2805	GLY	-	expression tag	UNP P42212
C	2806	HIS	-	expression tag	UNP P42212
C	2807	HIS	-	expression tag	UNP P42212
C	2808	HIS	-	expression tag	UNP P42212
C	2809	HIS	-	expression tag	UNP P42212
C	2810	HIS	-	expression tag	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	2811	HIS	-	expression tag	UNP P42212
C	2812	HIS	-	expression tag	UNP P42212
C	2813	HIS	-	expression tag	UNP P42212
C	2814	HIS	-	expression tag	UNP P42212
C	2815	HIS	-	expression tag	UNP P42212
B	2548	SER	-	linker	UNP E2JF22
B	2549	ASN	-	linker	UNP E2JF22
B	2550	SER	-	linker	UNP E2JF22
B	2551	LEU	-	linker	UNP E2JF22
B	2552	GLU	-	linker	UNP E2JF22
B	2553	VAL	-	linker	UNP E2JF22
B	2554	LEU	-	linker	UNP E2JF22
B	2555	PHE	-	linker	UNP E2JF22
B	2556	GLN	-	linker	UNP E2JF22
B	2557	GLY	-	linker	UNP E2JF22
B	2558	PRO	-	linker	UNP E2JF22
B	2559	THR	-	linker	UNP E2JF22
B	2560	ALA	-	linker	UNP E2JF22
B	2561	ALA	-	linker	UNP E2JF22
B	2562	ALA	-	linker	UNP E2JF22
B	2563	ALA	-	linker	UNP E2JF22
B	2564	VAL	-	linker	UNP E2JF22
B	2627	LEU	PHE	conflict	UNP P42212
B	2628	THR	SER	conflict	UNP P42212
B	2769	LYS	ALA	conflict	UNP P42212
B	2794	LEU	HIS	conflict	UNP P42212
B	2802	SER	-	expression tag	UNP P42212
B	2803	GLY	-	expression tag	UNP P42212
B	2804	GLY	-	expression tag	UNP P42212
B	2805	GLY	-	expression tag	UNP P42212
B	2806	HIS	-	expression tag	UNP P42212
B	2807	HIS	-	expression tag	UNP P42212
B	2808	HIS	-	expression tag	UNP P42212
B	2809	HIS	-	expression tag	UNP P42212
B	2810	HIS	-	expression tag	UNP P42212
B	2811	HIS	-	expression tag	UNP P42212
B	2812	HIS	-	expression tag	UNP P42212
B	2813	HIS	-	expression tag	UNP P42212
B	2814	HIS	-	expression tag	UNP P42212
B	2815	HIS	-	expression tag	UNP P42212

- Molecule 2 is a protein called Isoform I-mfA of MyoD family inhibitor.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	21	Total 148	C 86	N 21	O 33	S 8	0	0
2	D	21	Total 148	C 86	N 21	O 33	S 8	0	0
2	E	21	Total 148	C 86	N 21	O 33	S 8	0	0

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-22	MET	-	initiating methionine	UNP P70331
F	-21	ASP	-	expression tag	UNP P70331
F	-20	TYR	-	expression tag	UNP P70331
F	-19	LYS	-	expression tag	UNP P70331
F	-18	ASP	-	expression tag	UNP P70331
F	-17	ASP	-	expression tag	UNP P70331
F	-16	ASP	-	expression tag	UNP P70331
F	-15	ASP	-	expression tag	UNP P70331
F	-14	LYS	-	expression tag	UNP P70331
F	-13	GLY	-	expression tag	UNP P70331
F	-12	GLY	-	expression tag	UNP P70331
F	-11	GLY	-	expression tag	UNP P70331
F	-10	GLY	-	expression tag	UNP P70331
F	-9	SER	-	expression tag	UNP P70331
F	-8	SER	-	expression tag	UNP P70331
F	-7	THR	-	expression tag	UNP P70331
F	-6	THR	-	expression tag	UNP P70331
F	-5	ASN	-	expression tag	UNP P70331
F	-4	GLY	-	expression tag	UNP P70331
F	-3	SER	-	expression tag	UNP P70331
F	-2	SER	-	expression tag	UNP P70331
F	-1	ALA	-	expression tag	UNP P70331
F	0	THR	-	expression tag	UNP P70331
D	-22	MET	-	initiating methionine	UNP P70331
D	-21	ASP	-	expression tag	UNP P70331
D	-20	TYR	-	expression tag	UNP P70331
D	-19	LYS	-	expression tag	UNP P70331
D	-18	ASP	-	expression tag	UNP P70331
D	-17	ASP	-	expression tag	UNP P70331
D	-16	ASP	-	expression tag	UNP P70331
D	-15	ASP	-	expression tag	UNP P70331
D	-14	LYS	-	expression tag	UNP P70331
D	-13	GLY	-	expression tag	UNP P70331

Continued on next page...

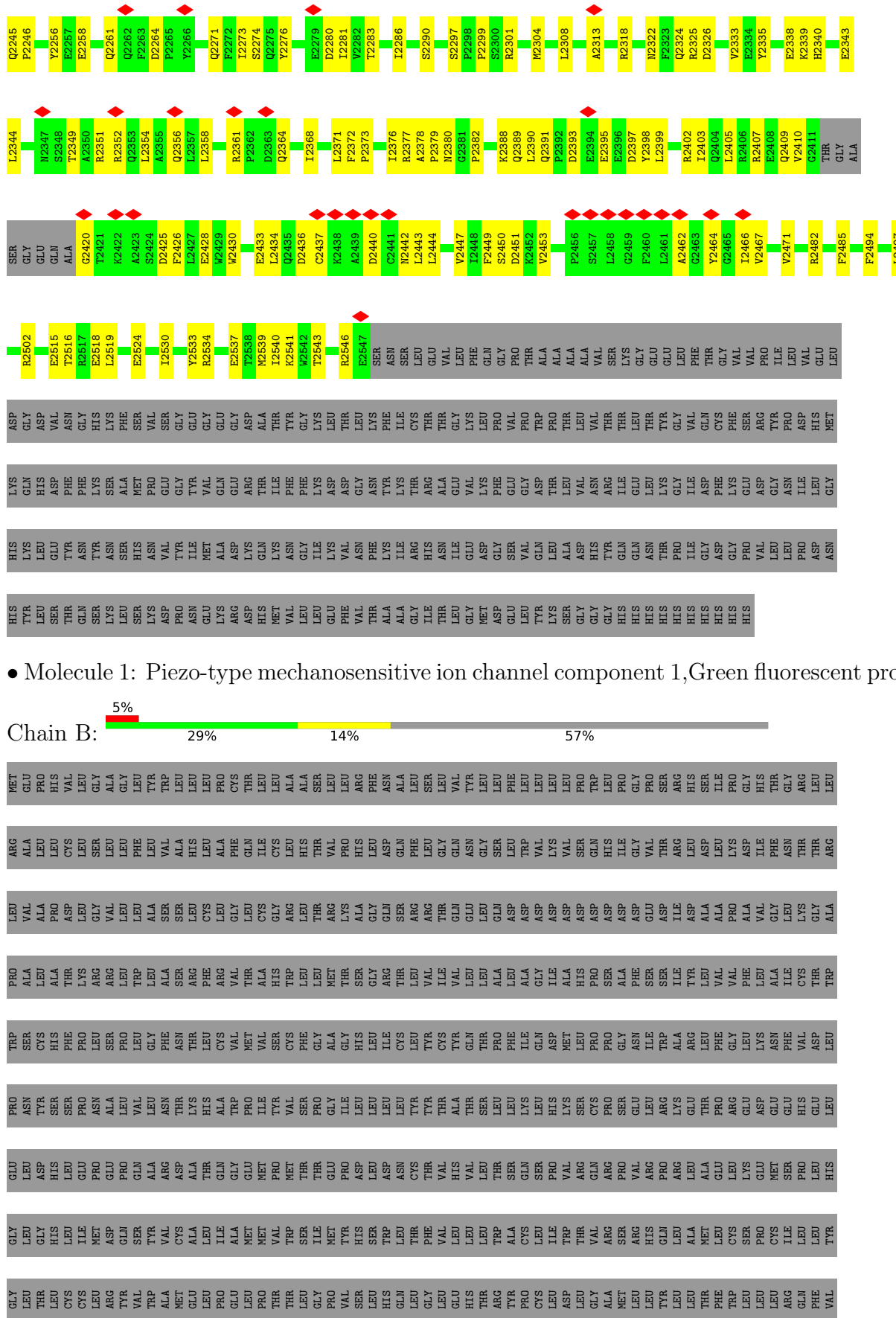
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	GLY	-	expression tag	UNP P70331
D	-11	GLY	-	expression tag	UNP P70331
D	-10	GLY	-	expression tag	UNP P70331
D	-9	SER	-	expression tag	UNP P70331
D	-8	SER	-	expression tag	UNP P70331
D	-7	THR	-	expression tag	UNP P70331
D	-6	THR	-	expression tag	UNP P70331
D	-5	ASN	-	expression tag	UNP P70331
D	-4	GLY	-	expression tag	UNP P70331
D	-3	SER	-	expression tag	UNP P70331
D	-2	SER	-	expression tag	UNP P70331
D	-1	ALA	-	expression tag	UNP P70331
D	0	THR	-	expression tag	UNP P70331
E	-22	MET	-	initiating methionine	UNP P70331
E	-21	ASP	-	expression tag	UNP P70331
E	-20	TYR	-	expression tag	UNP P70331
E	-19	LYS	-	expression tag	UNP P70331
E	-18	ASP	-	expression tag	UNP P70331
E	-17	ASP	-	expression tag	UNP P70331
E	-16	ASP	-	expression tag	UNP P70331
E	-15	ASP	-	expression tag	UNP P70331
E	-14	LYS	-	expression tag	UNP P70331
E	-13	GLY	-	expression tag	UNP P70331
E	-12	GLY	-	expression tag	UNP P70331
E	-11	GLY	-	expression tag	UNP P70331
E	-10	GLY	-	expression tag	UNP P70331
E	-9	SER	-	expression tag	UNP P70331
E	-8	SER	-	expression tag	UNP P70331
E	-7	THR	-	expression tag	UNP P70331
E	-6	THR	-	expression tag	UNP P70331
E	-5	ASN	-	expression tag	UNP P70331
E	-4	GLY	-	expression tag	UNP P70331
E	-3	SER	-	expression tag	UNP P70331
E	-2	SER	-	expression tag	UNP P70331
E	-1	ALA	-	expression tag	UNP P70331
E	0	THR	-	expression tag	UNP P70331

ASP	ARG	LEU	L784	D785	L786	A787	A788	S789	F790	S791	A792	V793	L794	T795	V799	R802	F810	V813	A814	L815	Y816	T817	V820	K823	E824	V827	M828	L831	L832	V833	V834	L835	F838	A839	P843	R844	F845	R846	P847	M848	A849	S850	C851	L852	S853	T854	V855	W856	T857							
C958	I959	I960	I961	V962	C963	K964	M965	L966	Y967	Q968	LEU	LYS	ILE	VAL	ASN	PRO	HIS	GLU	TTR	SER	ASN	CYS	THR	GLU	PRO	PHE	PRO	ASN	GLN	SER	LEU	LEU	TTR	ARG	GLY	PRO	VAL	ASP	PRO	ALA	ASN	TRP	PHE	GLY	VAL	ARG	LYS	GLY								
TTR	PRO	ASN	LEU	TRP	GLY	TTR	I924	L928	Q929	I930	L931	L932	L933	L934	V935	F936	E937	A938	V939	V940	Y941	Q944	E945	H946	Y947	R948	R949	Q950	H951	GLN	GLN	ALA	PRO	LEU	GLU	PRO	ALA	GLN	ALA	CYS	V873	L974	L975	S976	C977	N983	F984									
Y987	K988	E992	A998	V1001	I1002	M1007	F1008	M1009	V1010	H1013	W1016	L1017	I1020	R1024	R1025	R1026	E1027	A1028	I1029	A1030	R1031	L1032	W1033	P1034	M1035	Y1036	G1037	L1038	F1039	PRO	ALA	GLN	ALA	L1043	L1044	L1045	V1046	Q1047	Y1048	L1049	L1050	G1053	MET	PRO	PRO	ALA	LEU	CYS	ILE	ASP	TTR					
PRO	TRP	ARG	TRP	SER	LYS	ALA	ILE	PRO	M1072	N1073	A1075	L1076	I1077	K1078	W1079	L1080	Y1081	L1082	P1083	ASP	PHE	PHE	ARG	ALA	P1089	I1095	S1096	D1097	F1098	L1099	L1100	L1101	Q1109	V1110	A1113	E1117	E1118	W1119	Q1120	ARG	MET	ALA	GLY	ILE	ASN	THR	ASP	HIS	LEU	GLU	PRO	LEU				
R1134	P1137	M1138	P1139	N1140	P1141	N1142	F1143	R1147	S1148	Y1149	L1150	D1151	R1154	R1159	Y1160	V1165	F1170	G1173	I1179	Y1184	L1185	G1188	F1189	Y1190	L1191	L1198	L1199	Q1200	K1201	D1202	T1203	R1204	A1205	Q1206	L1207	V1208	W1209	D1211	L1214	M1217	V1220	L1227														
C1232	V1233	F1234	VAL	GLU	GLN	MET	GLN	GLN	ASN	PHE	C1243	I1246	L1251	VAL	CYS	THR	VAL	LYS	GLY	TTR	ASP	PRO	LYS	GLU	MET	THR	ARG	ASP	ASP	CYS	GLN	LEU	PRO	VAL	GLU	GLU	ALA	GLY	ILE	I1281	W1282	I1285	F1289	L1290	L1291	R1294	Y1301	H1304								
L1309	Q1315	R1318	G1319	F1320	A1321	L1322	N1324	A1325	A1326	K1329	H1334	R1335	G1336	L1337	E1338	Q1344	L1345	K1346	R1347	M1349	R1360	G1361	S1362	S1365	ARG	GLY	GLN	SER	LYS	ASP	PRO	GLN	ASP	PRO	GLN	GLY	PRO	GLY	PRO	ALA	ALA	GLN	THR	VAL	LEU	ARG	GLN	ARG	GLU							
PRO	ARG	GLN	TRP	ARG	PRO	TRP	LEU	H1403	Y1406	D1411	Y1412	F1413	D1418	S1419	E1420	F1421	GLU	GLU	ALA	LEU	PRO	GLU	ASP	PRO	ALA	ALA	GLN	SER	ALA	PHE	GLN	GLN	TRP	VAL	LEU	ASN	ALA	GLN	THR	VAL	GLY	ASP	PRO	VAL	PRO	ASP	GLY	GLU								
ARG	ALA	GLN	GLU	ARG	ALA	GLU	LEU	ALA	SER	GLY	ASP	LEU	ASN	PRO	ASP	VAL	PRO	GLU	ASP	GLU	GLU	MET	ALA	GLY	ARG	HIS	MET	MET	GLN	ARG	VAL	LEU	SER	THR	MET	GLN	VAL	GLY	PRO	VAL	LEU	G1509	Q1510	A1511	D1514	G1515	R1518	R1521								
A1522	F1523	T1524	K1525	R1528	T1529	M1530	S1531	D1532	V1533	L1534	E1537	R1538	Y1539	L1540	T1541	Q1542	Q1543	E1544	R1547	V1548	G1549	V1550	V1551	R1552	R1553	G1554	V1555	L1556	D1557	Q1558	L1559	TTR	VAL	GLY	GLU	ASP	GLU	ALA	THR	LEU	SER	GLU	PRO	VAL	GLU	VAL	G1509	Q1510	A1511	D1514	G1515	R1518	R1521			
LEU	GLY	ALA	GLU	PRO	LEU	SER	THR	ASP	THR	SER	SER	PRO	LEU	SER	THR	GLY	TYR	ASN	THR	ARG	SER	GLY	GLU	ILE	VAL	THR	ASP	ALA	GLY	ASP	GLY	LEU	GLN	ALA	VAL	GLY	SER	THR	ASP	GLU	LEU	LEU	LEU	LEU	LEU	VAL	GLU	ASN	ALA	ARG	THR	ARG	MET	LYS	ARG	THR
A1645	L1649	L1650	D1651	R1652	R1653	I1656	E1661	R1664	F1665	G1670	R1671	T1672	L1673	R1674	C1682	V1683	A1684	S1687	I1694	H1699	M1700	V1701	T1702	S1707	L1716	W1717	A1718	M1719	L1720	T1721	I1722	P1723	R1724	M1731	F1736	T1737	E1738	V1739	M1740	V1741	V1742	T1743	K1744	P1753	TRP											
ASN	SER	TTR	VAL	LEU	ARG	ARG	TTR	GLU	LYS	PRO	TTR	PHE	P1770	P1771	L1774	G1775	L1776	D1780	S1781	Y1782	I1783	K1784	L1787	Y1788	Q1789	L1790	M1791	H1796	Q1799	L1800	L1805	W1806	ASP	HIS	GLU	GLU	ASP	ARG	TYR	PRO	LYS	ASP	HIS	CYS	ARG	SER	SER	VAL	LYS	ASP	ARG					

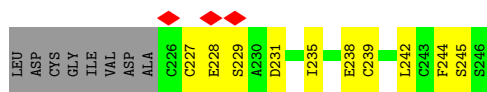












4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	56377	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.41	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.840	Depositor
Minimum map value	-1.588	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.34	Depositor
Map size (Å)	400.9, 400.9, 400.9	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.055, 1.055, 1.055	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	0.50	0/9876	0.59	0/13401
1	B	0.50	0/9876	0.59	0/13401
1	C	0.50	0/9876	0.59	0/13401
2	D	0.39	0/148	0.62	0/195
2	E	0.39	0/148	0.62	0/195
2	F	0.38	0/148	0.62	0/195
All	All	0.50	0/30072	0.59	0/40788

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9652	0	9495	358	0
1	B	9652	0	9495	361	0
1	C	9652	0	9495	344	0
2	D	148	0	130	9	0
2	E	148	0	130	12	0
2	F	148	0	130	12	0
All	All	29400	0	28875	1005	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 17.

All (1005) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1029:ILE:HA	1:A:1033:TRP:CD1	1.98	0.98
1:B:1029:ILE:HA	1:B:1033:TRP:CD1	1.97	0.98
1:C:1029:ILE:HA	1:C:1033:TRP:CD1	1.98	0.98
1:B:1118:GLU:HB3	1:B:1120:GLN:HG3	1.48	0.95
1:A:1118:GLU:HB3	1:A:1120:GLN:HG3	1.49	0.94
1:C:1118:GLU:HB3	1:C:1120:GLN:HG3	1.49	0.94
1:C:1559:LEU:HG	1:C:1653:ARG:HD2	1.56	0.88
1:A:2490:HIS:HD1	1:B:2494:PHE:HD2	1.16	0.88
1:C:1412:TYR:OH	1:B:2537:GLU:OE2	1.92	0.86
1:A:1559:LEU:HG	1:A:1653:ARG:HD2	1.56	0.85
1:B:1142:ASN:O	1:B:1147:ARG:NH2	2.09	0.85
1:B:1559:LEU:HG	1:B:1653:ARG:HD2	1.56	0.85
1:C:1142:ASN:O	1:C:1147:ARG:NH2	2.08	0.85
1:A:1142:ASN:O	1:A:1147:ARG:NH2	2.09	0.85
1:A:1687:SER:OG	1:A:1796:HIS:ND1	2.12	0.81
1:B:1687:SER:OG	1:B:1796:HIS:ND1	2.12	0.81
1:B:1029:ILE:HA	1:B:1033:TRP:HD1	1.45	0.81
1:C:1687:SER:OG	1:C:1796:HIS:ND1	2.12	0.81
1:C:1326:ALA:HA	1:C:1649:LEU:HD11	1.63	0.80
1:B:1326:ALA:HA	1:B:1649:LEU:HD11	1.63	0.80
1:A:2133:GLU:HG3	1:C:2485:PHE:HD2	1.47	0.79
1:A:2191:MET:HE1	2:D:238:GLU:HB3	1.63	0.79
1:C:2046:LYS:NZ	1:C:2093:SER:OG	2.14	0.79
1:A:2467:VAL:HG13	1:B:1996:TRP:CH2	2.18	0.78
1:A:1326:ALA:HA	1:A:1649:LEU:HD11	1.63	0.78
1:A:2492:ILE:HD11	1:B:2530:ILE:HD12	1.66	0.78
1:B:1002:ILE:HD13	1:B:1010:VAL:HG22	1.66	0.78
1:A:2333:VAL:HG21	1:A:2382:PRO:HG3	1.66	0.78
1:C:1002:ILE:HD13	1:C:1010:VAL:HG22	1.66	0.77
1:C:2333:VAL:HG21	1:C:2382:PRO:HG3	1.66	0.77
1:A:1002:ILE:HD13	1:A:1010:VAL:HG22	1.66	0.77
1:A:2018:GLN:OE1	1:C:2211:SER:OG	2.02	0.77
1:A:1029:ILE:HA	1:A:1033:TRP:HD1	1.45	0.77
1:A:2182:LYS:NZ	1:B:2144:ASP:HA	1.98	0.77
1:B:2333:VAL:HG21	1:B:2382:PRO:HG3	1.66	0.77
1:C:1029:ILE:HA	1:C:1033:TRP:HD1	1.45	0.76
1:A:2537:GLU:OE2	1:B:1412:TYR:OH	2.02	0.76
1:C:2113:LYS:O	1:C:2118:ASN:ND2	2.20	0.75
1:B:2113:LYS:O	1:B:2118:ASN:ND2	2.20	0.75
1:A:2046:LYS:NZ	1:A:2093:SER:OG	2.14	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2046:LYS:NZ	1:B:2093:SER:OG	2.14	0.74
1:A:1684:ALA:O	1:A:1799:GLN:NE2	2.18	0.74
1:A:2113:LYS:O	1:A:2118:ASN:ND2	2.20	0.74
1:A:2211:SER:HB2	1:B:1995:PHE:HZ	1.51	0.74
1:A:2420:GLY:N	1:A:2425:ASP:OD2	2.21	0.74
1:B:2420:GLY:N	1:B:2425:ASP:OD2	2.20	0.74
1:C:2420:GLY:N	1:C:2425:ASP:OD2	2.21	0.74
1:B:2407:ARG:NH2	1:B:2428:GLU:OE2	2.21	0.73
1:C:2407:ARG:NH2	1:C:2428:GLU:OE2	2.21	0.73
1:A:2407:ARG:NH2	1:A:2428:GLU:OE2	2.21	0.72
1:B:2313:ALA:O	1:B:2351:ARG:NH2	2.23	0.72
1:A:2179:LYS:HE2	1:B:1406:VAL:HG21	1.72	0.72
1:C:2313:ALA:O	1:C:2351:ARG:NH2	2.23	0.72
1:B:1684:ALA:O	1:B:1799:GLN:NE2	2.18	0.71
1:C:1684:ALA:O	1:C:1799:GLN:NE2	2.18	0.71
1:A:2313:ALA:O	1:A:2351:ARG:NH2	2.23	0.71
1:A:2493:MET:HA	1:B:2534:ARG:HG3	1.73	0.70
1:C:2069:THR:HG22	1:C:2070:GLU:H	1.57	0.70
1:A:2133:GLU:HG3	1:C:2485:PHE:CD2	2.27	0.69
1:B:2069:THR:HG22	1:B:2070:GLU:H	1.57	0.69
1:C:2235:TYR:HD1	1:C:2304:MET:HG3	1.58	0.69
1:C:1246:ILE:HG13	1:C:1251:LEU:HB2	1.74	0.69
1:B:2191:MET:HE1	2:E:238:GLU:HB3	1.73	0.69
1:A:1246:ILE:HG13	1:A:1251:LEU:HB2	1.74	0.69
1:B:1550:GLU:HG3	1:B:1551:VAL:HG12	1.75	0.69
1:A:1550:GLU:HG3	1:A:1551:VAL:HG12	1.75	0.68
1:B:1246:ILE:HG13	1:B:1251:LEU:HB2	1.74	0.68
1:A:2211:SER:HB2	1:B:1995:PHE:CZ	2.28	0.68
1:A:2069:THR:HG22	1:A:2070:GLU:H	1.57	0.68
1:A:2318:ARG:HE	1:A:2339:LYS:HE3	1.59	0.68
1:C:1203:THR:O	1:C:1207:LEU:HB2	1.94	0.68
1:A:2283:THR:HG22	1:A:2447:VAL:HG22	1.76	0.68
1:B:1117:GLU:HG2	1:B:1118:GLU:HG2	1.76	0.68
1:A:2235:TYR:HD1	1:A:2304:MET:HG3	1.58	0.68
1:C:2283:THR:HG22	1:C:2447:VAL:HG22	1.76	0.68
1:B:1203:THR:O	1:B:1207:LEU:HB2	1.94	0.68
1:A:2108:ASN:HB3	1:A:2111:THR:HG22	1.76	0.68
1:B:2283:THR:HG22	1:B:2447:VAL:HG22	1.76	0.67
1:C:1550:GLU:HG3	1:C:1551:VAL:HG12	1.75	0.67
1:A:1117:GLU:HG2	1:A:1118:GLU:HG2	1.76	0.67
1:C:1731:MET:HE3	1:C:1806:TRP:HZ2	1.58	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2235:TYR:HD1	1:B:2304:MET:HG3	1.58	0.67
1:A:1731:MET:HE3	1:A:1806:TRP:HZ2	1.58	0.67
1:B:1731:MET:HE3	1:B:1806:TRP:HZ2	1.58	0.67
1:A:1984:ASP:HB3	1:A:2031:MET:HE2	1.77	0.67
1:C:2318:ARG:HE	1:C:2339:LYS:HE3	1.59	0.67
1:B:2108:ASN:HB3	1:B:2111:THR:HG22	1.76	0.67
1:B:2304:MET:HE2	1:B:2358:LEU:HD22	1.76	0.67
1:C:1117:GLU:HG2	1:C:1118:GLU:HG2	1.76	0.67
1:B:2318:ARG:HE	1:B:2339:LYS:HE3	1.59	0.66
1:A:1203:THR:O	1:A:1207:LEU:HB2	1.94	0.66
1:A:1345:LEU:HD12	1:A:2104:ARG:HE	1.60	0.66
1:C:2021:LEU:HD11	1:B:2208:LEU:HA	1.77	0.66
1:C:2304:MET:HE2	1:C:2358:LEU:HD22	1.76	0.66
1:A:845:PHE:O	1:A:849:ALA:N	2.27	0.66
1:C:1724:ARG:NH2	1:C:1805:LEU:O	2.29	0.66
1:C:2105:ILE:HG13	1:C:2106:LEU:HD12	1.77	0.66
1:A:1724:ARG:NH2	1:A:1805:LEU:O	2.29	0.66
1:C:1032:LEU:HG	1:C:1036:TYR:HB2	1.77	0.66
1:C:1984:ASP:HB3	1:C:2031:MET:HE2	1.77	0.66
1:A:1994:GLY:HA3	1:A:2078:VAL:HG11	1.78	0.66
1:A:2105:ILE:HG13	1:A:2106:LEU:HD12	1.77	0.66
1:B:1994:GLY:HA3	1:B:2078:VAL:HG11	1.78	0.66
1:B:1032:LEU:HG	1:B:1036:TYR:HB2	1.77	0.66
1:B:1724:ARG:NH2	1:B:1805:LEU:O	2.29	0.66
1:C:2108:ASN:HB3	1:C:2111:THR:HG22	1.76	0.66
1:C:2108:ASN:OD1	1:C:2109:PHE:N	2.29	0.66
1:C:1345:LEU:HD12	1:C:2104:ARG:HE	1.60	0.66
1:C:1994:GLY:HA3	1:C:2078:VAL:HG11	1.78	0.65
1:A:1148:SER:OG	1:A:1151:ASP:OD2	2.13	0.65
1:A:2108:ASN:OD1	1:A:2109:PHE:N	2.29	0.65
1:C:2123:GLN:HG2	2:F:244:PHE:CD2	2.31	0.65
1:B:1345:LEU:HD12	1:B:2104:ARG:HE	1.60	0.65
1:A:1032:LEU:HG	1:A:1036:TYR:HB2	1.77	0.65
1:A:2128:VAL:HG11	1:A:2131:LEU:HD12	1.79	0.65
1:A:2235:TYR:CD1	1:A:2304:MET:HG3	2.32	0.65
1:A:2304:MET:HE2	1:A:2358:LEU:HD22	1.77	0.65
1:C:2530:ILE:HD12	1:B:2492:ILE:HD11	1.77	0.65
1:B:1984:ASP:HB3	1:B:2031:MET:HE2	1.77	0.65
1:B:2105:ILE:HG13	1:B:2106:LEU:HD12	1.77	0.65
1:B:2356:GLN:O	1:B:2364:GLN:NE2	2.29	0.65
1:B:2373:PRO:HB2	1:B:2376:ILE:HD11	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1996:TRP:CH2	1:B:2467:VAL:HG13	2.32	0.65
1:C:2356:GLN:O	1:C:2364:GLN:NE2	2.29	0.65
1:B:2108:ASN:OD1	1:B:2109:PHE:N	2.29	0.65
1:A:2373:PRO:HB2	1:A:2376:ILE:HD11	1.79	0.65
1:A:2191:MET:CE	2:D:238:GLU:HB3	2.27	0.65
1:C:1246:ILE:HA	1:C:1251:LEU:HD23	1.79	0.65
1:A:2356:GLN:O	1:A:2364:GLN:NE2	2.29	0.64
1:B:2235:TYR:CD1	1:B:2304:MET:HG3	2.32	0.64
1:C:2128:VAL:HG11	1:C:2131:LEU:HD12	1.79	0.64
1:C:2235:TYR:CD1	1:C:2304:MET:HG3	2.32	0.64
1:B:845:PHE:O	1:B:849:ALA:N	2.28	0.64
1:C:2373:PRO:HB2	1:C:2376:ILE:HD11	1.79	0.64
1:B:1246:ILE:HA	1:B:1251:LEU:HD23	1.80	0.64
1:A:2133:GLU:OE1	1:C:2482:ARG:NE	2.17	0.64
1:C:1020:ILE:HA	1:C:1033:TRP:HH2	1.62	0.64
1:B:1020:ILE:HA	1:B:1033:TRP:HH2	1.62	0.64
1:A:1020:ILE:HA	1:A:1033:TRP:HH2	1.62	0.64
1:B:2533:TYR:CE1	1:B:2539:MET:HE1	2.33	0.64
1:C:2533:TYR:CE1	1:C:2539:MET:HE1	2.33	0.64
1:B:1159:ARG:HG2	1:B:1160:TYR:CD1	2.34	0.63
1:C:1159:ARG:HG2	1:C:1160:TYR:CD1	2.34	0.63
1:C:2123:GLN:HG2	2:F:244:PHE:HD2	1.64	0.63
1:A:2533:TYR:CE1	1:A:2539:MET:HE1	2.33	0.63
1:B:2128:VAL:HG11	1:B:2131:LEU:HD12	1.79	0.63
1:A:1246:ILE:HA	1:A:1251:LEU:HD23	1.80	0.63
1:B:1661:GLU:OE1	1:B:1664:ARG:NH1	2.31	0.63
1:B:2198:PHE:CZ	1:B:2202:ILE:HD11	2.34	0.63
1:A:1661:GLU:OE1	1:A:1664:ARG:NH1	2.31	0.62
1:A:1159:ARG:HG2	1:A:1160:TYR:CD1	2.34	0.62
1:A:2123:GLN:HG2	2:D:244:PHE:HD2	1.64	0.62
1:C:2184:LYS:NZ	2:F:231:ASP:OD1	2.27	0.62
1:C:1661:GLU:OE1	1:C:1664:ARG:NH1	2.31	0.62
1:C:2198:PHE:CZ	1:C:2202:ILE:HD11	2.34	0.62
1:B:1148:SER:OG	1:B:1151:ASP:OD2	2.14	0.62
1:A:2182:LYS:HZ3	1:B:2144:ASP:HA	1.63	0.62
1:A:2198:PHE:CZ	1:A:2202:ILE:HD11	2.34	0.61
1:C:845:PHE:O	1:C:849:ALA:N	2.28	0.61
1:B:2377:ARG:NH1	1:B:2451:ASP:OD2	2.33	0.61
1:B:1722:ILE:HG23	1:B:1723:PRO:HD2	1.82	0.61
1:C:2191:MET:HE1	2:F:238:GLU:HB3	1.83	0.61
1:C:2377:ARG:NH1	1:C:2451:ASP:OD2	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2377:ARG:NH1	1:A:2451:ASP:OD2	2.33	0.61
1:A:2021:LEU:HD11	1:C:2208:LEU:HA	1.83	0.60
1:B:2041:LYS:HG3	1:B:2105:ILE:HD13	1.84	0.60
1:A:1722:ILE:HG23	1:A:1723:PRO:HD2	1.82	0.60
1:A:2030:THR:HG23	1:A:2049:PHE:HZ	1.66	0.60
1:A:2208:LEU:HA	1:B:2021:LEU:HD11	1.83	0.60
1:A:2271:GLN:O	1:A:2274:SER:OG	2.20	0.60
1:C:1995:PHE:HZ	1:B:2211:SER:HB2	1.66	0.60
1:C:1722:ILE:HG23	1:C:1723:PRO:HD2	1.82	0.60
1:C:2041:LYS:HG3	1:C:2105:ILE:HD13	1.84	0.60
1:A:2372:PHE:HD2	1:A:2434:LEU:HD21	1.67	0.59
1:C:2372:PHE:HD2	1:C:2434:LEU:HD21	1.67	0.59
1:C:2497:LEU:HD21	1:C:2539:MET:HE2	1.84	0.59
1:B:2497:LEU:HD21	1:B:2539:MET:HE2	1.84	0.59
1:A:1671:ARG:HG3	1:A:1672:THR:HG23	1.84	0.59
1:A:2182:LYS:HZ2	1:B:2144:ASP:HA	1.65	0.59
1:B:2030:THR:HG23	1:B:2049:PHE:HZ	1.66	0.59
1:C:1315:GLN:HE21	1:C:1537:GLU:HB2	1.67	0.59
1:C:2030:THR:HG23	1:C:2049:PHE:HZ	1.66	0.59
1:B:2191:MET:CE	2:E:238:GLU:HB3	2.33	0.59
1:A:1020:ILE:HD11	1:A:1040:LEU:HD12	1.85	0.59
1:A:1315:GLN:HE21	1:A:1537:GLU:HB2	1.67	0.59
1:A:1521:ARG:HE	1:A:1528:ARG:CZ	2.16	0.59
1:A:2301:ARG:NH2	1:A:2358:LEU:O	2.35	0.59
1:C:1134:ARG:HG3	1:C:1137:PRO:HG3	1.85	0.59
1:B:1671:ARG:HG3	1:B:1672:THR:HG23	1.84	0.59
1:B:1134:ARG:HG3	1:B:1137:PRO:HG3	1.85	0.59
1:B:1315:GLN:HE21	1:B:1537:GLU:HB2	1.68	0.59
1:B:1521:ARG:HE	1:B:1528:ARG:CZ	2.16	0.59
1:A:2497:LEU:HD21	1:A:2539:MET:HE2	1.84	0.59
1:C:1671:ARG:HG3	1:C:1672:THR:HG23	1.84	0.59
1:B:2372:PHE:HD2	1:B:2434:LEU:HD21	1.67	0.59
1:B:1020:ILE:HD11	1:B:1040:LEU:HD12	1.85	0.59
1:B:2301:ARG:NH2	1:B:2358:LEU:O	2.35	0.58
1:A:1141:PRO:HB2	1:A:1304:HIS:ND1	2.19	0.58
1:C:1521:ARG:HE	1:C:1528:ARG:CZ	2.16	0.58
1:C:2378:ALA:N	1:C:2449:PHE:O	2.36	0.58
1:A:2210:MET:HE3	1:A:2466:ILE:HG23	1.85	0.58
1:A:2485:PHE:CG	1:B:2153:MET:HE2	2.38	0.58
1:C:1020:ILE:HD11	1:C:1040:LEU:HD12	1.85	0.58
1:A:1134:ARG:HG3	1:A:1137:PRO:HG3	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1141:PRO:HB2	1:B:1304:HIS:ND1	2.19	0.58
1:B:2210:MET:HE3	1:B:2466:ILE:HG23	1.85	0.58
1:A:2041:LYS:HG3	1:A:2105:ILE:HD13	1.84	0.58
1:C:2410:VAL:HG12	1:C:2426:PHE:HA	1.86	0.58
1:A:2021:LEU:HD23	1:C:2204:TRP:HE1	1.67	0.58
1:B:2123:GLN:HG2	2:E:244:PHE:CD2	2.39	0.58
1:C:1141:PRO:HB2	1:C:1304:HIS:ND1	2.19	0.58
1:B:2271:GLN:O	1:B:2274:SER:OG	2.20	0.57
1:A:2390:LEU:HD11	1:A:2449:PHE:HE2	1.69	0.57
1:C:1109:GLN:O	1:C:1113:ALA:HB3	2.04	0.57
1:B:1143:PHE:CE1	1:B:1154:LYS:HD3	2.39	0.57
1:A:1702:THR:HB	1:A:1784:LYS:HD2	1.86	0.57
1:B:1025:ARG:O	1:B:1029:ILE:HG12	2.05	0.57
1:B:2123:GLN:HG2	2:E:244:PHE:HD2	1.69	0.57
1:A:2021:LEU:HD23	1:C:2204:TRP:NE1	2.20	0.57
1:C:2271:GLN:O	1:C:2274:SER:OG	2.20	0.57
1:C:2301:ARG:NH2	1:C:2358:LEU:O	2.35	0.57
1:A:1143:PHE:CE1	1:A:1154:LYS:HD3	2.39	0.57
1:B:2390:LEU:HD11	1:B:2449:PHE:HE2	1.70	0.57
1:C:2165:ILE:HD11	2:F:245:SER:OG	2.04	0.57
1:C:2390:LEU:HD11	1:C:2449:PHE:HE2	1.69	0.57
1:B:1318:ARG:NH2	1:B:1537:GLU:OE1	2.38	0.57
1:A:1109:GLN:O	1:A:1113:ALA:HB3	2.04	0.57
1:C:1025:ARG:O	1:C:1029:ILE:HG12	2.05	0.57
1:C:2210:MET:HE3	1:C:2466:ILE:HG23	1.85	0.57
1:B:1109:GLN:O	1:B:1113:ALA:HB3	2.04	0.57
1:A:1165:VAL:HG22	1:A:1289:PHE:HB3	1.87	0.56
1:C:1143:PHE:CE1	1:C:1154:LYS:HD3	2.39	0.56
1:B:2378:ALA:N	1:B:2449:PHE:O	2.36	0.56
1:A:1996:TRP:CH2	1:C:2467:VAL:HG13	2.40	0.56
1:C:1148:SER:OG	1:C:1151:ASP:OD2	2.13	0.56
1:C:1315:GLN:NE2	1:C:1537:GLU:HB2	2.21	0.56
1:C:1318:ARG:NH2	1:C:1537:GLU:OE1	2.38	0.56
1:B:1702:THR:HB	1:B:1784:LYS:HD2	1.86	0.56
1:B:2410:VAL:HG12	1:B:2426:PHE:HA	1.86	0.56
1:A:2407:ARG:HD3	1:A:2426:PHE:HE2	1.71	0.56
1:B:2407:ARG:HD3	1:B:2426:PHE:HE2	1.71	0.56
1:A:2378:ALA:N	1:A:2449:PHE:O	2.36	0.56
1:A:2402:ARG:N	1:A:2433:GLU:O	2.25	0.56
1:B:1555:VAL:HA	1:B:1558:GLN:CD	2.31	0.56
1:A:1008:PHE:HB3	1:A:1080:LEU:HD13	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1025:ARG:O	1:A:1029:ILE:HG12	2.05	0.56
1:A:1406:VAL:HG21	1:C:2179:LYS:HE2	1.87	0.56
1:A:1555:VAL:HA	1:A:1558:GLN:CD	2.31	0.56
1:B:1409:SER:O	1:B:1409:SER:OG	2.22	0.56
1:A:2410:VAL:HG12	1:A:2426:PHE:HA	1.86	0.56
1:C:1555:VAL:HA	1:C:1558:GLN:CD	2.31	0.56
1:B:1315:GLN:NE2	1:B:1537:GLU:HB2	2.21	0.56
1:C:1702:THR:HB	1:C:1784:LYS:HD2	1.86	0.56
1:C:2349:THR:HA	1:C:2352:ARG:HH22	1.71	0.56
1:A:2390:LEU:HD11	1:A:2449:PHE:CE2	2.42	0.55
1:C:1719:MET:O	1:C:1720:LEU:HD23	2.06	0.55
1:A:1318:ARG:NH2	1:A:1537:GLU:OE1	2.38	0.55
1:A:1719:MET:O	1:A:1720:LEU:HD23	2.06	0.55
1:C:1008:PHE:HB3	1:C:1080:LEU:HD13	1.87	0.55
1:C:2018:GLN:OE1	1:B:2211:SER:OG	2.24	0.55
1:C:2391:GLN:HB2	1:C:2397:ASP:HB2	1.88	0.55
1:A:1522:ALA:HA	1:A:1525:LYS:HD3	1.88	0.55
1:C:2390:LEU:HD11	1:C:2449:PHE:CE2	2.42	0.55
1:C:2407:ARG:HD3	1:C:2426:PHE:HE2	1.71	0.55
1:C:992:GLU:HG3	1:C:1291:LEU:CD2	2.36	0.55
1:B:1008:PHE:HB3	1:B:1080:LEU:HD13	1.88	0.55
1:C:1165:VAL:HG22	1:C:1289:PHE:HB3	1.87	0.55
1:C:2308:LEU:HD13	1:C:2354:LEU:HB3	1.89	0.55
1:A:992:GLU:HG3	1:A:1291:LEU:CD2	2.36	0.55
1:B:992:GLU:HG3	1:B:1291:LEU:CD2	2.36	0.55
1:B:1165:VAL:HG22	1:B:1289:PHE:HB3	1.87	0.55
1:A:1315:GLN:NE2	1:A:1537:GLU:HB2	2.21	0.55
1:B:1150:LEU:HD11	1:B:1154:LYS:HE3	1.88	0.55
1:B:1522:ALA:HA	1:B:1525:LYS:HD3	1.88	0.55
1:B:2390:LEU:HD11	1:B:2449:PHE:CE2	2.42	0.55
1:C:1522:ALA:HA	1:C:1525:LYS:HD3	1.89	0.55
1:C:1969:LYS:HD3	1:C:1970:TYR:N	2.22	0.54
1:B:1969:LYS:HD3	1:B:1970:TYR:N	2.22	0.54
1:B:2308:LEU:HD13	1:B:2354:LEU:HB3	1.89	0.54
1:A:2391:GLN:HB2	1:A:2397:ASP:HB2	1.88	0.54
1:C:1001:VAL:HG21	1:C:1013:HIS:ND1	2.22	0.54
1:C:1150:LEU:HD11	1:C:1154:LYS:HE3	1.89	0.54
1:A:1138:ASN:ND2	1:A:1141:PRO:HB3	2.22	0.54
1:A:1150:LEU:HD11	1:A:1154:LYS:HE3	1.89	0.54
1:A:2192:GLY:HA3	1:B:2141:VAL:HG21	1.88	0.54
1:A:2349:THR:HA	1:A:2352:ARG:HH22	1.71	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1701:VAL:HG12	1:C:1784:LYS:HD3	1.89	0.54
1:A:2308:LEU:HD13	1:A:2354:LEU:HB3	1.89	0.54
1:C:1138:ASN:ND2	1:C:1141:PRO:HB3	2.22	0.54
1:B:1170:PHE:CD1	1:B:1787:LEU:HD13	2.43	0.54
1:A:2485:PHE:CD2	1:B:2153:MET:HE2	2.42	0.54
1:A:1170:PHE:CD1	1:A:1787:LEU:HD13	2.42	0.54
1:A:1969:LYS:HD3	1:A:1970:TYR:N	2.22	0.54
1:A:2523:GLU:OE2	1:C:2180:GLY:HA2	2.07	0.54
1:C:2494:PHE:HD2	1:B:2490:HIS:HD1	1.52	0.54
1:B:1551:VAL:HG22	1:B:1554:GLY:H	1.73	0.54
1:B:1701:VAL:HG12	1:B:1784:LYS:HD3	1.89	0.54
1:B:2349:THR:HA	1:B:2352:ARG:HH22	1.71	0.54
1:C:1170:PHE:CD1	1:C:1787:LEU:HD13	2.42	0.54
1:B:2368:ILE:HD12	1:B:2403:ILE:HD12	1.90	0.54
2:E:227:CYS:SG	2:E:228:GLU:N	2.81	0.54
1:B:1001:VAL:HG21	1:B:1013:HIS:ND1	2.22	0.54
1:A:2184:LYS:HB2	1:A:2187:VAL:HG12	1.89	0.54
1:A:2290:SER:O	1:A:2290:SER:OG	2.25	0.54
1:C:1141:PRO:O	1:C:1143:PHE:N	2.40	0.54
1:C:2184:LYS:HB2	1:C:2187:VAL:HG12	1.89	0.54
1:C:2402:ARG:N	1:C:2433:GLU:O	2.25	0.54
1:A:1001:VAL:HG21	1:A:1013:HIS:ND1	2.22	0.54
1:C:1044:LEU:HB3	1:C:1101:LEU:HD13	1.90	0.54
1:B:1719:MET:O	1:B:1720:LEU:HD23	2.06	0.54
1:A:2104:ARG:HD3	1:A:2515:GLU:OE1	2.08	0.53
1:C:1551:VAL:HG22	1:C:1554:GLY:H	1.73	0.53
1:C:2497:LEU:HD23	1:C:2543:THR:HG21	1.90	0.53
1:B:1008:PHE:HB2	1:B:1079:TRP:CH2	2.44	0.53
1:B:2391:GLN:HB2	1:B:2397:ASP:HB2	1.88	0.53
1:A:1141:PRO:O	1:A:1143:PHE:N	2.40	0.53
1:A:1551:VAL:HG22	1:A:1554:GLY:H	1.73	0.53
1:A:1701:VAL:HG12	1:A:1784:LYS:HD3	1.89	0.53
1:A:2204:TRP:CE2	1:B:2025:LEU:HD12	2.43	0.53
1:B:2497:LEU:HD23	1:B:2543:THR:HG21	1.90	0.53
2:F:227:CYS:SG	2:F:228:GLU:N	2.81	0.53
1:A:1008:PHE:HB2	1:A:1079:TRP:CH2	2.44	0.53
1:C:1029:ILE:CA	1:C:1033:TRP:HD1	2.19	0.53
1:B:1184:TYR:OH	1:B:1217:ASN:OD1	2.26	0.53
1:B:1771:PRO:O	1:B:1775:GLY:N	2.42	0.53
1:B:2184:LYS:HB2	1:B:2187:VAL:HG12	1.89	0.53
1:B:1007:ASN:HD21	1:B:1009:MET:HB3	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1670:GLY:HA2	1:B:1674:ARG:HG3	1.91	0.53
1:B:2104:ARG:HD3	1:B:2515:GLU:OE1	2.08	0.53
2:D:227:CYS:SG	2:D:228:GLU:N	2.81	0.53
1:C:1007:ASN:HD21	1:C:1009:MET:HB3	1.73	0.53
1:B:1699:HIS:NE2	1:B:2062:PHE:CE2	2.77	0.53
1:A:1044:LEU:HB3	1:A:1101:LEU:HD13	1.90	0.53
1:A:1184:TYR:OH	1:A:1217:ASN:OD1	2.26	0.53
1:A:2256:TYR:OH	1:A:2273:ILE:O	2.26	0.53
1:C:1020:ILE:HG23	1:C:1033:TRP:CZ3	2.44	0.53
1:C:1771:PRO:O	1:C:1775:GLY:N	2.42	0.53
1:C:2133:GLU:HG3	1:B:2485:PHE:HD2	1.74	0.53
1:B:1044:LEU:HB3	1:B:1101:LEU:HD13	1.90	0.53
1:B:1320:PHE:O	1:B:1324:ASN:ND2	2.42	0.53
1:B:2340:HIS:O	1:B:2340:HIS:ND1	2.42	0.53
1:A:1007:ASN:HD21	1:A:1009:MET:HB3	1.73	0.53
1:A:2040:ARG:NH2	1:A:2142:TRP:O	2.42	0.53
1:A:2544:ARG:NH1	1:B:1411:ASP:OD1	2.41	0.53
1:C:1008:PHE:HB2	1:C:1079:TRP:CH2	2.44	0.53
1:C:2340:HIS:O	1:C:2340:HIS:ND1	2.42	0.53
1:B:1138:ASN:ND2	1:B:1141:PRO:HB3	2.22	0.53
1:A:1699:HIS:NE2	1:A:2062:PHE:CE2	2.77	0.53
1:A:1771:PRO:O	1:A:1775:GLY:N	2.42	0.53
1:C:1320:PHE:O	1:C:1324:ASN:ND2	2.42	0.53
1:C:2368:ILE:HD12	1:C:2403:ILE:HD12	1.90	0.52
1:A:1320:PHE:O	1:A:1324:ASN:ND2	2.42	0.52
1:A:1403:HIS:HB2	1:C:2178:PRO:O	2.09	0.52
1:A:2368:ILE:HD12	1:A:2403:ILE:HD12	1.90	0.52
1:A:2497:LEU:HD23	1:A:2543:THR:HG21	1.90	0.52
1:C:1184:TYR:OH	1:C:1217:ASN:OD1	2.26	0.52
1:C:2040:ARG:NH2	1:C:2142:TRP:O	2.42	0.52
1:C:2464:TYR:HA	1:C:2467:VAL:HB	1.91	0.52
1:A:1142:ASN:HA	1:A:1304:HIS:CE1	2.45	0.52
1:A:1344:GLN:OE1	1:A:1347:ARG:NH2	2.35	0.52
1:B:2497:LEU:H	1:B:2497:LEU:HD12	1.74	0.52
1:B:2516:THR:O	1:B:2516:THR:HG22	2.10	0.52
1:B:1141:PRO:O	1:B:1143:PHE:N	2.40	0.52
1:B:2140:TRP:CD1	1:B:2145:THR:HG21	2.45	0.52
1:C:1409:SER:O	1:C:1409:SER:OG	2.22	0.52
1:C:1670:GLY:HA2	1:C:1674:ARG:HG3	1.91	0.52
1:C:2191:MET:CE	2:F:238:GLU:HB3	2.39	0.52
1:B:1533:VAL:O	1:B:1537:GLU:HG3	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1743:THR:HG22	1:B:1776:LEU:HD11	1.92	0.52
1:B:2464:TYR:HA	1:B:2467:VAL:HB	1.91	0.52
1:B:1020:ILE:HG23	1:B:1033:TRP:CZ3	2.44	0.52
1:B:2040:ARG:NH2	1:B:2142:TRP:O	2.42	0.52
1:A:1029:ILE:CA	1:A:1033:TRP:HD1	2.19	0.52
1:A:2231:LYS:NZ	1:B:2244:GLN:HE22	2.08	0.52
1:B:1029:ILE:CA	1:B:1033:TRP:HD1	2.18	0.52
1:B:1109:GLN:O	1:B:1113:ALA:CB	2.58	0.52
1:A:1020:ILE:HG23	1:A:1033:TRP:CZ3	2.44	0.52
1:C:1533:VAL:O	1:C:1537:GLU:HG3	2.10	0.52
1:C:1699:HIS:NE2	1:C:2062:PHE:CE2	2.77	0.52
1:C:2058:HIS:NE2	1:C:2083:TYR:OH	2.32	0.52
1:C:2104:ARG:HD3	1:C:2515:GLU:OE1	2.08	0.52
1:B:1724:ARG:HH22	1:B:1805:LEU:H	1.57	0.52
1:A:1670:GLY:HA2	1:A:1674:ARG:HG3	1.91	0.51
1:A:2140:TRP:CD1	1:A:2145:THR:HG21	2.45	0.51
1:A:2340:HIS:ND1	1:A:2340:HIS:O	2.42	0.51
1:A:2490:HIS:HA	1:B:2494:PHE:CE2	2.45	0.51
1:A:2497:LEU:HD12	1:A:2497:LEU:H	1.75	0.51
1:B:1035:ASN:O	1:B:1038:LEU:HB3	2.11	0.51
1:B:2290:SER:O	1:B:2290:SER:OG	2.25	0.51
1:C:1961:PHE:O	1:C:1965:ILE:HG13	2.11	0.51
1:C:2516:THR:HG22	1:C:2516:THR:O	2.09	0.51
1:B:1961:PHE:O	1:B:1965:ILE:HG13	2.11	0.51
1:B:2402:ARG:N	1:B:2433:GLU:O	2.25	0.51
1:C:1142:ASN:HA	1:C:1304:HIS:CE1	2.45	0.51
1:B:2256:TYR:OH	1:B:2273:ILE:O	2.26	0.51
1:A:1724:ARG:HH22	1:A:1805:LEU:H	1.57	0.51
1:A:2225:ASP:HB3	1:A:2324:GLN:HB3	1.92	0.51
1:C:984:PHE:HB3	1:C:987:TYR:HB3	1.93	0.51
1:A:984:PHE:HB3	1:A:987:TYR:HB3	1.93	0.51
1:A:2123:GLN:HG2	2:D:244:PHE:CD2	2.44	0.51
1:C:2497:LEU:HD12	1:C:2497:LEU:H	1.74	0.51
1:B:1142:ASN:HA	1:B:1304:HIS:CE1	2.45	0.51
1:A:2516:THR:HG22	1:A:2516:THR:O	2.09	0.51
1:C:1109:GLN:O	1:C:1113:ALA:CB	2.58	0.51
1:C:2140:TRP:CD1	1:C:2145:THR:HG21	2.45	0.51
1:C:2225:ASP:HB3	1:C:2324:GLN:HB3	1.92	0.51
1:A:1035:ASN:O	1:A:1038:LEU:HB3	2.11	0.51
1:A:1109:GLN:O	1:A:1113:ALA:CB	2.58	0.51
1:A:1533:VAL:O	1:A:1537:GLU:HG3	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:967:ARG:N	1:C:1120:GLN:HB3	2.26	0.51
1:C:973:ASP:O	1:C:976:SER:OG	2.22	0.51
1:A:1044:LEU:CB	1:A:1101:LEU:HD13	2.41	0.51
1:B:1736:PHE:CE2	1:B:1740:MET:HE2	2.46	0.51
1:A:1360:ARG:NH2	1:A:2524:GLU:OE2	2.44	0.51
1:A:1736:PHE:CE2	1:A:1740:MET:HE2	2.46	0.51
1:C:1736:PHE:CE2	1:C:1740:MET:HE2	2.46	0.51
1:B:967:ARG:N	1:B:1120:GLN:HB3	2.26	0.51
1:B:1360:ARG:NH2	1:B:2524:GLU:OE2	2.44	0.51
1:B:2148:SER:OG	1:B:2149:LEU:N	2.44	0.51
1:A:1743:THR:HG22	1:A:1776:LEU:HD11	1.92	0.51
1:C:1724:ARG:HH22	1:C:1805:LEU:H	1.57	0.51
1:C:2191:MET:HE1	2:F:239:CYS:N	2.26	0.51
1:B:984:PHE:HB3	1:B:987:TYR:HB3	1.93	0.51
1:B:2225:ASP:HB3	1:B:2324:GLN:HB3	1.92	0.51
1:A:1201:LYS:O	1:A:1206:GLN:NE2	2.44	0.50
1:A:1961:PHE:O	1:A:1965:ILE:HG13	2.10	0.50
1:A:2148:SER:OG	1:A:2149:LEU:N	2.44	0.50
1:C:1731:MET:HE3	1:C:1806:TRP:CZ2	2.43	0.50
1:B:1044:LEU:CB	1:B:1101:LEU:HD13	2.41	0.50
1:A:2464:TYR:HA	1:A:2467:VAL:HB	1.91	0.50
1:C:1360:ARG:NH2	1:C:2524:GLU:OE2	2.44	0.50
1:C:1743:THR:HG22	1:C:1776:LEU:HD11	1.92	0.50
1:B:1201:LYS:O	1:B:1206:GLN:NE2	2.44	0.50
1:A:967:ARG:N	1:A:1120:GLN:HB3	2.26	0.50
1:A:2490:HIS:ND1	1:B:2494:PHE:HD2	1.98	0.50
1:C:2227:THR:HB	1:C:2322:ASN:HB3	1.93	0.50
1:A:2235:TYR:HE1	1:A:2304:MET:HA	1.77	0.50
1:A:2409:GLN:NE2	1:A:2410:VAL:O	2.44	0.50
1:C:2256:TYR:OH	1:C:2273:ILE:O	2.26	0.50
1:A:2030:THR:HG23	1:A:2049:PHE:CZ	2.47	0.50
1:B:2235:TYR:HE1	1:B:2304:MET:HA	1.77	0.50
1:B:2373:PRO:HB3	1:B:2398:TYR:CE1	2.47	0.50
1:C:1035:ASN:O	1:C:1038:LEU:HB3	2.11	0.50
1:C:2235:TYR:HE1	1:C:2304:MET:HA	1.77	0.50
1:B:1651:ASP:O	1:B:1652:ARG:NH1	2.45	0.50
1:B:1731:MET:HE3	1:B:1806:TRP:CZ2	2.43	0.50
1:C:2409:GLN:NE2	1:C:2410:VAL:O	2.44	0.50
1:C:1044:LEU:CB	1:C:1101:LEU:HD13	2.41	0.49
1:B:1987:ASP:OD1	1:B:2082:TRP:NE1	2.45	0.49
1:A:1651:ASP:O	1:A:1652:ARG:NH1	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1987:ASP:OD1	1:A:2082:TRP:NE1	2.45	0.49
1:A:2244:GLN:HG2	1:A:2245:GLN:N	2.28	0.49
1:B:2244:GLN:HG2	1:B:2245:GLN:N	2.27	0.49
1:A:974:LEU:HG	1:A:975:LEU:HD12	1.94	0.49
1:C:2244:GLN:HG2	1:C:2245:GLN:N	2.28	0.49
1:C:2373:PRO:HB3	1:C:2398:TYR:CE1	2.47	0.49
1:B:2409:GLN:NE2	1:B:2410:VAL:O	2.44	0.49
1:C:2534:ARG:HG3	1:B:2493:MET:HA	1.93	0.49
1:A:2325:ARG:NH2	1:A:2379:PRO:O	2.46	0.49
1:A:2467:VAL:HG13	1:B:1996:TRP:CZ3	2.48	0.49
1:C:2030:THR:HG23	1:C:2049:PHE:CZ	2.47	0.49
1:B:2325:ARG:NH2	1:B:2379:PRO:O	2.46	0.49
1:A:1013:HIS:HE2	1:A:1047:GLN:NE2	2.10	0.49
1:A:1412:TYR:OH	1:C:2537:GLU:OE2	2.23	0.49
1:A:2227:THR:HB	1:A:2322:ASN:HB3	1.93	0.49
1:A:2373:PRO:HB3	1:A:2398:TYR:CE1	2.47	0.49
1:C:1651:ASP:O	1:C:1652:ARG:NH1	2.45	0.49
1:B:974:LEU:HG	1:B:975:LEU:HD12	1.94	0.49
1:B:1694:ILE:HG21	1:B:1789:GLN:HA	1.95	0.49
1:B:2227:THR:HB	1:B:2322:ASN:HB3	1.93	0.49
1:A:1074:SER:O	1:A:1077:ILE:HG22	2.13	0.49
1:C:1782:TYR:CE2	1:C:1783:ILE:HG23	2.48	0.49
1:C:2211:SER:O	1:C:2215:SER:OG	2.31	0.49
1:C:1016:TRP:CZ2	1:C:1043:PHE:HE2	2.31	0.49
1:C:1995:PHE:CZ	1:B:2211:SER:HB2	2.46	0.49
1:C:2325:ARG:NH2	1:C:2379:PRO:O	2.46	0.49
1:A:1016:TRP:CZ2	1:A:1043:PHE:HE2	2.31	0.48
1:C:974:LEU:HG	1:C:975:LEU:HD12	1.94	0.48
1:C:2133:GLU:OE1	1:B:2482:ARG:NE	2.29	0.48
1:C:2191:MET:HE1	2:F:238:GLU:C	2.38	0.48
1:B:1013:HIS:HE2	1:B:1047:GLN:NE2	2.10	0.48
1:B:1344:GLN:OE1	1:B:1347:ARG:NH2	2.35	0.48
1:B:2485:PHE:HE1	2:E:242:LEU:HD11	1.78	0.48
1:C:1013:HIS:HE2	1:C:1047:GLN:NE2	2.10	0.48
1:C:1026:ARG:O	1:C:1029:ILE:HB	2.13	0.48
1:C:1987:ASP:OD1	1:C:2082:TRP:NE1	2.46	0.48
1:C:2393:ASP:C	1:C:2395:GLU:H	2.21	0.48
1:B:1026:ARG:O	1:B:1029:ILE:HB	2.13	0.48
1:B:1074:SER:O	1:B:1077:ILE:HG22	2.13	0.48
1:B:2295:ARG:HD3	1:B:2295:ARG:HA	1.63	0.48
1:A:1782:TYR:CE2	1:A:1783:ILE:HG23	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2191:MET:HE1	2:D:238:GLU:C	2.38	0.48
1:C:1074:SER:O	1:C:1077:ILE:HG22	2.13	0.48
1:B:1521:ARG:HB3	1:B:1528:ARG:NH2	2.28	0.48
1:A:1031:ARG:HD2	1:A:1032:LEU:HB2	1.95	0.48
1:C:2130:PHE:HA	1:C:2133:GLU:OE2	2.13	0.48
1:B:1142:ASN:HA	1:B:1304:HIS:NE2	2.29	0.48
1:A:2130:PHE:HA	1:A:2133:GLU:OE2	2.14	0.48
1:C:1362:SER:O	1:C:1365:SER:OG	2.31	0.48
1:C:1406:VAL:HG21	1:B:2179:LYS:HE2	1.94	0.48
1:C:1521:ARG:HB3	1:C:1528:ARG:NH2	2.28	0.48
1:C:2148:SER:OG	1:C:2149:LEU:N	2.44	0.48
1:B:1362:SER:O	1:B:1365:SER:OG	2.31	0.48
1:B:1787:LEU:O	1:B:1791:MET:HG2	2.14	0.48
1:A:1694:ILE:HG21	1:A:1789:GLN:HA	1.95	0.48
1:A:2281:ILE:HD13	1:A:2449:PHE:CE1	2.49	0.48
1:C:1189:PHE:HZ	1:C:1741:VAL:HG11	1.79	0.48
1:C:1344:GLN:OE1	1:C:1347:ARG:NH2	2.35	0.48
1:B:1159:ARG:HG2	1:B:1160:TYR:HD1	1.77	0.48
1:B:1198:LEU:HD11	1:B:1209:LEU:HD23	1.96	0.48
1:A:1026:ARG:O	1:A:1029:ILE:HB	2.13	0.48
1:C:1142:ASN:HA	1:C:1304:HIS:NE2	2.29	0.48
1:C:1198:LEU:HD11	1:C:1209:LEU:HD23	1.96	0.48
1:C:1791:MET:HE3	1:C:1791:MET:HA	1.96	0.48
1:B:2244:GLN:HG2	1:B:2245:GLN:H	1.79	0.48
1:A:1521:ARG:HB3	1:A:1528:ARG:NH2	2.28	0.48
1:A:2295:ARG:HD3	1:A:2295:ARG:HA	1.63	0.48
1:C:1694:ILE:HG21	1:C:1789:GLN:HA	1.95	0.48
1:A:1142:ASN:HA	1:A:1304:HIS:NE2	2.29	0.48
1:B:1214:ILE:HG12	1:B:1290:LEU:HG	1.96	0.48
1:A:2261:GLN:HA	1:A:2264:ASP:OD1	2.14	0.47
1:B:1699:HIS:NE2	1:B:2062:PHE:HE2	2.12	0.47
1:B:1791:MET:HE3	1:B:1791:MET:HA	1.96	0.47
1:B:2130:PHE:HA	1:B:2133:GLU:OE2	2.13	0.47
1:B:2211:SER:O	1:B:2215:SER:OG	2.31	0.47
1:A:2352:ARG:NH1	1:A:2352:ARG:HB3	2.29	0.47
1:C:1787:LEU:O	1:C:1791:MET:HG2	2.14	0.47
1:C:2261:GLN:HA	1:C:2264:ASP:OD1	2.14	0.47
1:B:1143:PHE:HZ	1:B:1301:TYR:CD2	2.32	0.47
1:B:1189:PHE:HZ	1:B:1741:VAL:HG11	1.79	0.47
1:A:2393:ASP:C	1:A:2395:GLU:H	2.22	0.47
1:A:2467:VAL:HG22	1:B:1996:TRP:CE2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1699:HIS:NE2	1:A:2062:PHE:HE2	2.13	0.47
1:A:2492:ILE:HD11	1:B:2530:ILE:CD1	2.42	0.47
1:C:2281:ILE:HD13	1:C:2449:PHE:CE1	2.49	0.47
1:B:1016:TRP:CZ2	1:B:1043:PHE:HE2	2.31	0.47
1:B:1179:ILE:HG23	1:B:1179:ILE:O	2.15	0.47
1:B:1329:LYS:HD3	1:B:1649:LEU:HD12	1.96	0.47
1:B:1782:TYR:CE2	1:B:1783:ILE:HG23	2.48	0.47
1:A:1143:PHE:HZ	1:A:1301:TYR:CD2	2.32	0.47
1:A:1170:PHE:HB2	1:A:1188:CYS:SG	2.55	0.47
1:A:1179:ILE:HG23	1:A:1179:ILE:O	2.14	0.47
1:A:1538:ARG:O	1:A:1542:THR:HG23	2.15	0.47
1:A:1787:LEU:O	1:A:1791:MET:HG2	2.14	0.47
1:A:1791:MET:HE3	1:A:1791:MET:HA	1.96	0.47
1:C:1031:ARG:HD2	1:C:1032:LEU:HB2	1.96	0.47
1:C:1170:PHE:HB2	1:C:1188:CYS:SG	2.55	0.47
1:C:2244:GLN:HG2	1:C:2245:GLN:H	1.79	0.47
1:C:2352:ARG:NH1	1:C:2352:ARG:HB3	2.29	0.47
1:B:2462:ALA:HA	1:B:2466:ILE:HG22	1.96	0.47
1:A:1159:ARG:HG2	1:A:1160:TYR:HD1	1.77	0.47
1:A:1198:LEU:HD11	1:A:1209:LEU:HD23	1.96	0.47
1:A:1329:LYS:HD3	1:A:1649:LEU:HD12	1.97	0.47
1:B:1031:ARG:HD2	1:B:1032:LEU:HB2	1.95	0.47
1:B:1744:LYS:HB2	1:B:1744:LYS:HE2	1.74	0.47
1:B:2030:THR:HG23	1:B:2049:PHE:CZ	2.47	0.47
1:B:2281:ILE:HD13	1:B:2449:PHE:CE1	2.49	0.47
1:A:1214:ILE:HG12	1:A:1290:LEU:HG	1.97	0.47
1:A:1731:MET:HE3	1:A:1806:TRP:CZ2	2.43	0.47
1:A:2131:LEU:HA	1:A:2131:LEU:HD23	1.69	0.47
1:C:987:TYR:OH	1:C:1119:TRP:HA	2.15	0.47
1:C:1179:ILE:O	1:C:1179:ILE:HG23	2.14	0.47
1:C:1200:GLN:HE22	1:C:1309:LEU:HB3	1.80	0.47
1:C:1329:LYS:HD3	1:C:1649:LEU:HD12	1.97	0.47
1:C:1699:HIS:NE2	1:C:2062:PHE:HE2	2.13	0.47
1:C:2410:VAL:H	1:C:2426:PHE:HB3	1.80	0.47
1:C:2462:ALA:HA	1:C:2466:ILE:HG22	1.96	0.47
1:B:1716:LEU:HA	1:B:1716:LEU:HD23	1.63	0.47
1:B:2131:LEU:O	1:B:2135:ARG:HB3	2.15	0.47
1:B:2187:VAL:HG23	2:E:235:ILE:HG12	1.97	0.47
1:B:2261:GLN:HA	1:B:2264:ASP:OD1	2.14	0.47
1:B:2352:ARG:HB3	1:B:2352:ARG:NH1	2.29	0.47
1:B:2410:VAL:H	1:B:2426:PHE:HB3	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1189:PHE:HZ	1:A:1741:VAL:HG11	1.79	0.47
1:A:2462:ALA:HA	1:A:2466:ILE:HG22	1.96	0.47
1:C:1200:GLN:NE2	1:C:1309:LEU:HB3	2.30	0.47
1:A:2211:SER:O	1:A:2215:SER:OG	2.31	0.47
1:B:1170:PHE:HB2	1:B:1188:CYS:SG	2.55	0.47
1:B:2393:ASP:C	1:B:2395:GLU:H	2.22	0.47
1:B:2440:ASP:OD1	1:B:2440:ASP:N	2.48	0.47
1:A:1200:GLN:NE2	1:A:1309:LEU:HB3	2.30	0.46
1:A:1362:SER:O	1:A:1365:SER:OG	2.31	0.46
1:C:1020:ILE:HA	1:C:1033:TRP:CH2	2.48	0.46
1:C:2502:ARG:HH21	1:C:2546:ARG:HD3	1.80	0.46
1:B:987:TYR:OH	1:B:1119:TRP:HA	2.15	0.46
1:B:1200:GLN:NE2	1:B:1309:LEU:HB3	2.30	0.46
1:A:2244:GLN:HG2	1:A:2245:GLN:H	1.79	0.46
1:C:1538:ARG:O	1:C:1542:THR:HG23	2.15	0.46
1:C:2133:GLU:HG3	1:B:2485:PHE:CD2	2.49	0.46
1:C:2485:PHE:HE1	2:F:242:LEU:HD11	1.80	0.46
1:B:1538:ARG:O	1:B:1542:THR:HG23	2.15	0.46
1:B:1699:HIS:ND1	1:B:1707:SER:O	2.48	0.46
1:A:1744:LYS:HB2	1:A:1744:LYS:HE2	1.73	0.46
1:A:2534:ARG:O	1:C:2540:ILE:HD11	2.15	0.46
1:C:2219:VAL:N	1:C:2453:VAL:O	2.47	0.46
1:A:973:ASP:O	1:A:976:SER:OG	2.22	0.46
1:A:2131:LEU:O	1:A:2135:ARG:HB3	2.15	0.46
1:A:2219:VAL:N	1:A:2453:VAL:O	2.47	0.46
1:A:2440:ASP:HB2	1:A:2443:LEU:HB2	1.98	0.46
1:C:1214:ILE:HG12	1:C:1290:LEU:HG	1.97	0.46
1:C:2440:ASP:HB2	1:C:2443:LEU:HB2	1.98	0.46
1:B:987:TYR:HA	1:B:1110:VAL:HG11	1.98	0.46
1:A:987:TYR:OH	1:A:1119:TRP:HA	2.15	0.46
1:A:2033:ILE:O	1:A:2037:LEU:HD23	2.16	0.46
1:C:1143:PHE:HZ	1:C:1301:TYR:CD2	2.32	0.46
1:B:2140:TRP:CE3	1:B:2149:LEU:HD13	2.51	0.46
1:A:1724:ARG:HH22	1:A:1805:LEU:N	2.14	0.46
1:A:2245:GLN:HB3	1:A:2246:PRO:CD	2.46	0.46
1:B:1724:ARG:HH22	1:B:1805:LEU:N	2.14	0.46
1:A:1524:THR:HG21	1:A:1682:CYS:HA	1.98	0.46
1:A:2410:VAL:H	1:A:2426:PHE:HB3	1.80	0.46
1:A:2425:ASP:HB3	1:A:2426:PHE:HD1	1.81	0.46
1:C:1159:ARG:HG2	1:C:1160:TYR:HD1	1.77	0.46
1:C:1201:LYS:O	1:C:1206:GLN:NE2	2.44	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1699:HIS:ND1	1:C:1707:SER:O	2.48	0.46
1:C:2140:TRP:CE3	1:C:2149:LEU:HD13	2.51	0.46
1:C:2425:ASP:HB3	1:C:2426:PHE:HD1	1.81	0.46
1:C:2131:LEU:O	1:C:2135:ARG:HB3	2.15	0.46
1:A:1699:HIS:ND1	1:A:1707:SER:O	2.48	0.46
1:A:2224:ILE:HD13	1:A:2326:ASP:HB3	1.98	0.46
1:A:2490:HIS:ND1	1:B:2494:PHE:CD2	2.62	0.46
1:A:2516:THR:O	1:A:2518:GLU:N	2.49	0.46
1:C:2290:SER:O	1:C:2290:SER:OG	2.25	0.46
1:B:1984:ASP:HB3	1:B:2031:MET:CE	2.45	0.46
1:B:2149:LEU:HA	1:B:2149:LEU:HD12	1.69	0.46
1:B:2516:THR:O	1:B:2518:GLU:N	2.49	0.46
1:B:2516:THR:C	1:B:2518:GLU:H	2.24	0.46
1:A:2498:PRO:HD3	1:B:2534:ARG:NH2	2.31	0.45
1:C:1984:ASP:HB3	1:C:2031:MET:CE	2.45	0.45
1:C:2033:ILE:O	1:C:2037:LEU:HD23	2.16	0.45
1:C:2442:ASN:OD1	1:C:2442:ASN:N	2.49	0.45
1:B:1232:CYS:SG	1:B:1233:VAL:HG23	2.57	0.45
1:B:1524:THR:HG21	1:B:1682:CYS:HA	1.98	0.45
1:B:1670:GLY:O	1:B:1674:ARG:NH2	2.49	0.45
1:B:2502:ARG:HH21	1:B:2546:ARG:HD3	1.80	0.45
1:A:1191:LEU:HD23	1:A:1191:LEU:HA	1.79	0.45
1:C:1969:LYS:HD3	1:C:1970:TYR:C	2.42	0.45
1:B:1200:GLN:HE22	1:B:1309:LEU:HB3	1.80	0.45
1:B:1328:LEU:HD23	1:B:1328:LEU:HA	1.85	0.45
1:A:1008:PHE:HB2	1:A:1079:TRP:CZ3	2.51	0.45
1:A:2502:ARG:HH21	1:A:2546:ARG:HD3	1.80	0.45
1:C:998:ALA:O	1:C:1001:VAL:HG22	2.17	0.45
1:C:1217:ASN:O	1:C:1220:VAL:HG12	2.17	0.45
1:C:2516:THR:O	1:C:2518:GLU:N	2.49	0.45
1:B:2245:GLN:HB3	1:B:2246:PRO:CD	2.46	0.45
1:A:2516:THR:C	1:A:2518:GLU:H	2.24	0.45
1:C:1008:PHE:HB2	1:C:1079:TRP:CZ3	2.51	0.45
1:C:1189:PHE:CD1	1:C:1738:GLU:HG3	2.52	0.45
1:C:1724:ARG:HH22	1:C:1805:LEU:N	2.14	0.45
1:A:1189:PHE:CD1	1:A:1738:GLU:HG3	2.51	0.45
1:A:1670:GLY:O	1:A:1674:ARG:NH2	2.49	0.45
1:A:1969:LYS:HD3	1:A:1970:TYR:C	2.41	0.45
1:B:1969:LYS:HD3	1:B:1970:TYR:C	2.42	0.45
1:B:2207:LEU:HD12	1:B:2207:LEU:HA	1.77	0.45
1:B:2440:ASP:HB2	1:B:2443:LEU:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:988:LYS:HD3	1:A:988:LYS:HA	1.76	0.45
1:A:998:ALA:O	1:A:1001:VAL:HG22	2.17	0.45
1:A:1984:ASP:CB	1:A:2031:MET:HE2	2.46	0.45
1:A:2140:TRP:CE3	1:A:2149:LEU:HD13	2.51	0.45
1:A:2429:TRP:CE2	1:C:2297:SER:HB2	2.52	0.45
1:C:987:TYR:HA	1:C:1110:VAL:HG11	1.98	0.45
1:B:2425:ASP:HB3	1:B:2426:PHE:HD1	1.81	0.45
1:A:1227:LEU:HD23	1:A:1227:LEU:HA	1.80	0.45
1:C:1670:GLY:O	1:C:1674:ARG:NH2	2.50	0.45
1:B:1008:PHE:HB2	1:B:1079:TRP:CZ3	2.51	0.45
1:B:1189:PHE:CD1	1:B:1738:GLU:HG3	2.51	0.45
1:B:1217:ASN:O	1:B:1220:VAL:HG12	2.17	0.45
1:A:1027:GLU:HG2	1:A:1028:ALA:N	2.32	0.45
1:C:1232:CYS:SG	1:C:1233:VAL:HG23	2.57	0.45
1:C:2245:GLN:HB3	1:C:2246:PRO:CD	2.46	0.45
1:A:987:TYR:HA	1:A:1110:VAL:HG11	1.98	0.45
1:C:2191:MET:HG3	1:C:2195:ILE:HD12	1.99	0.45
1:C:2516:THR:C	1:C:2518:GLU:H	2.24	0.45
1:B:2224:ILE:HD13	1:B:2326:ASP:HB3	1.98	0.45
1:A:2434:LEU:HB2	1:A:2437:CYS:SG	2.57	0.45
1:C:1774:LEU:HD12	1:C:1774:LEU:HA	1.70	0.45
1:B:1349:MET:HE1	1:B:2516:THR:HB	1.99	0.45
1:B:2434:LEU:HB2	1:B:2437:CYS:SG	2.57	0.45
1:C:1170:PHE:CE1	1:C:1787:LEU:HB2	2.52	0.44
1:B:998:ALA:O	1:B:1002:ILE:HG12	2.17	0.44
1:B:1020:ILE:HA	1:B:1033:TRP:CH2	2.48	0.44
1:B:1191:LEU:HD23	1:B:1191:LEU:HA	1.79	0.44
1:B:2033:ILE:O	1:B:2037:LEU:HD23	2.16	0.44
1:B:2035:ARG:HH12	1:B:2109:PHE:HZ	1.65	0.44
2:F:228:GLU:HG2	2:F:229:SER:H	1.82	0.44
1:A:1349:MET:HE1	1:A:2516:THR:HB	1.99	0.44
1:A:2245:GLN:OE1	1:A:2245:GLN:HA	2.18	0.44
1:C:1007:ASN:HB2	1:C:1079:TRP:O	2.18	0.44
1:C:1349:MET:HE1	1:C:2516:THR:HB	1.99	0.44
1:B:2058:HIS:NE2	1:B:2083:TYR:OH	2.32	0.44
1:A:1200:GLN:HE22	1:A:1309:LEU:HB3	1.80	0.44
1:A:1411:ASP:HB3	1:A:1413:PHE:CD2	2.53	0.44
1:A:1984:ASP:HB3	1:A:2031:MET:CE	2.45	0.44
1:C:1282:TRP:HA	1:C:1285:ILE:HG22	1.99	0.44
1:C:2245:GLN:OE1	1:C:2245:GLN:HA	2.17	0.44
1:C:2443:LEU:HD23	1:C:2443:LEU:HA	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2165:ILE:HD11	2:E:245:SER:OG	2.17	0.44
1:B:2184:LYS:NZ	2:E:231:ASP:OD1	2.31	0.44
1:A:1701:VAL:CG1	1:A:1784:LYS:HD3	2.48	0.44
1:C:1027:GLU:HG2	1:C:1028:ALA:N	2.32	0.44
1:C:1524:THR:HG21	1:C:1682:CYS:HA	1.98	0.44
1:C:2434:LEU:HB2	1:C:2437:CYS:SG	2.57	0.44
1:B:1217:ASN:HA	1:B:1220:VAL:HG12	1.99	0.44
1:B:1411:ASP:HB3	1:B:1413:PHE:CD2	2.53	0.44
1:A:1217:ASN:HA	1:A:1220:VAL:HG12	1.99	0.44
1:A:2442:ASN:OD1	1:A:2442:ASN:N	2.50	0.44
1:B:1027:GLU:HG2	1:B:1028:ALA:N	2.32	0.44
1:B:2388:LYS:HB3	1:B:2389:GLN:NE2	2.32	0.44
1:A:1232:CYS:SG	1:A:1233:VAL:HG23	2.57	0.44
1:A:1774:LEU:HD12	1:A:1774:LEU:HA	1.71	0.44
1:A:2191:MET:HG3	1:A:2195:ILE:HD12	1.99	0.44
1:B:1322:LEU:HD22	1:B:1530:MET:HG3	1.99	0.44
1:B:2108:ASN:HB3	1:B:2111:THR:CG2	2.47	0.44
1:B:2191:MET:HG3	1:B:2195:ILE:HD12	1.99	0.44
1:B:2219:VAL:N	1:B:2453:VAL:O	2.47	0.44
2:E:228:GLU:HG2	2:E:229:SER:H	1.82	0.44
1:A:2519:LEU:HD23	1:A:2519:LEU:HA	1.77	0.44
1:C:2224:ILE:HD13	1:C:2326:ASP:HB3	1.99	0.44
1:B:1080:LEU:HG	1:B:1082:LEU:HD23	2.00	0.44
1:A:1217:ASN:O	1:A:1220:VAL:HG12	2.17	0.44
1:A:1322:LEU:HD22	1:A:1530:MET:HG3	1.99	0.44
1:C:998:ALA:O	1:C:1002:ILE:HG12	2.18	0.44
1:C:2388:LYS:HB3	1:C:2389:GLN:NE2	2.33	0.44
2:D:228:GLU:HG2	2:D:229:SER:H	1.82	0.44
1:A:2035:ARG:HH12	1:A:2109:PHE:HZ	1.65	0.44
1:C:1217:ASN:HA	1:C:1220:VAL:HG12	1.99	0.44
1:C:1716:LEU:HD23	1:C:1716:LEU:HA	1.63	0.44
1:C:2436:ASP:OD1	1:C:2436:ASP:N	2.51	0.44
1:B:998:ALA:O	1:B:1001:VAL:HG22	2.17	0.44
1:B:1243:CYS:O	1:B:1246:ILE:HG22	2.18	0.44
1:B:1984:ASP:CB	1:B:2031:MET:HE2	2.46	0.44
1:A:998:ALA:O	1:A:1002:ILE:HG12	2.18	0.43
1:A:1007:ASN:HB2	1:A:1079:TRP:O	2.18	0.43
1:A:1080:LEU:HG	1:A:1082:LEU:HD23	2.00	0.43
1:A:1170:PHE:CE1	1:A:1787:LEU:HB2	2.52	0.43
1:A:1243:CYS:O	1:A:1246:ILE:HG22	2.18	0.43
1:A:1971:ARG:HD2	1:A:2098:ARG:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1411:ASP:HB3	1:C:1413:PHE:CD2	2.53	0.43
1:B:973:ASP:O	1:B:976:SER:OG	2.22	0.43
1:B:1701:VAL:CG1	1:B:1784:LYS:HD3	2.48	0.43
1:B:2228:VAL:HG21	1:B:2286:ILE:HD13	2.00	0.43
1:A:2137:VAL:O	1:A:2141:VAL:HG23	2.18	0.43
1:A:2541:LYS:O	1:A:2541:LYS:HG2	2.18	0.43
1:C:2352:ARG:HB3	1:C:2352:ARG:CZ	2.48	0.43
1:B:1170:PHE:CE1	1:B:1787:LEU:HB2	2.53	0.43
1:B:2436:ASP:OD1	1:B:2436:ASP:N	2.51	0.43
1:A:1552:ARG:HD3	1:A:1553:ARG:HH22	1.83	0.43
1:A:2062:PHE:O	1:A:2066:PRO:HG2	2.19	0.43
1:A:2276:TYR:CE1	1:A:2449:PHE:HB3	2.54	0.43
1:C:2228:VAL:HG21	1:C:2286:ILE:HD13	2.00	0.43
1:B:1007:ASN:HB2	1:B:1079:TRP:O	2.18	0.43
1:A:2228:VAL:HG21	1:A:2286:ILE:HD13	2.00	0.43
1:A:2238:LEU:HD23	1:A:2430:TRP:CD2	2.54	0.43
1:C:2276:TYR:CE1	1:C:2449:PHE:HB3	2.54	0.43
1:B:1282:TRP:HA	1:B:1285:ILE:HG22	1.99	0.43
1:B:2442:ASN:OD1	1:B:2442:ASN:N	2.49	0.43
1:A:1097:ASP:OD1	1:A:1098:PHE:N	2.52	0.43
1:A:2191:MET:HE1	2:D:238:GLU:CB	2.42	0.43
1:A:2529:LEU:HA	1:A:2529:LEU:HD12	1.81	0.43
1:C:1335:ARG:HH22	1:C:1971:ARG:H	1.67	0.43
1:B:1204:ARG:HA	1:B:1204:ARG:HD2	1.88	0.43
1:B:2062:PHE:O	1:B:2066:PRO:HG2	2.18	0.43
1:A:2371:LEU:N	1:A:2399:LEU:O	2.47	0.43
1:A:2388:LYS:HB3	1:A:2389:GLN:NE2	2.33	0.43
1:C:2153:MET:HE2	1:B:2485:PHE:CG	2.53	0.43
1:B:2238:LEU:HD23	1:B:2430:TRP:CD2	2.54	0.43
1:B:2245:GLN:HA	1:B:2245:GLN:OE1	2.17	0.43
1:B:2352:ARG:HB3	1:B:2352:ARG:CZ	2.48	0.43
1:A:2280:ASP:O	1:A:2450:SER:OG	2.37	0.43
1:C:1552:ARG:HD3	1:C:1553:ARG:HH22	1.83	0.43
1:B:1097:ASP:OD1	1:B:1098:PHE:N	2.52	0.43
1:B:1971:ARG:HD2	1:B:2098:ARG:O	2.19	0.43
1:B:2361:ARG:HH11	1:B:2364:GLN:CD	2.27	0.43
1:A:1744:LYS:NZ	1:A:1775:GLY:O	2.52	0.43
1:A:2343:GLU:O	1:A:2344:LEU:HD23	2.19	0.43
1:C:1243:CYS:O	1:C:1246:ILE:HG22	2.18	0.43
1:C:1971:ARG:HD2	1:C:2098:ARG:O	2.18	0.43
1:C:2244:GLN:N	1:C:2244:GLN:OE1	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2525:LEU:HA	1:B:2525:LEU:HD23	1.76	0.43
1:A:1020:ILE:HA	1:A:1033:TRP:CH2	2.48	0.43
1:A:2361:ARG:HH11	1:A:2364:GLN:CD	2.27	0.43
1:C:1331:ILE:HD13	1:C:1331:ILE:HA	1.89	0.43
1:C:1540:LEU:HA	1:C:1543:GLN:HG2	2.01	0.43
1:C:1985:ILE:HD13	1:C:1985:ILE:HA	1.92	0.43
1:C:2062:PHE:O	1:C:2066:PRO:HG2	2.19	0.43
1:C:2092:LEU:HD23	1:C:2092:LEU:HA	1.76	0.43
1:C:2380:ASN:OD1	1:C:2453:VAL:HG22	2.19	0.43
1:B:970:LEU:HD12	1:B:977:CYS:HA	2.01	0.43
1:A:1991:ILE:HD11	1:A:2082:TRP:HE1	1.83	0.43
1:A:2149:LEU:HD12	1:A:2149:LEU:HA	1.70	0.43
1:A:2179:LYS:HA	1:B:1402:ASP:O	2.19	0.43
1:A:2467:VAL:HG22	1:B:1996:TRP:CD2	2.54	0.43
1:C:1080:LEU:HG	1:C:1082:LEU:HD23	2.00	0.43
1:C:1701:VAL:CG1	1:C:1784:LYS:HD3	2.48	0.43
1:C:2238:LEU:HD23	1:C:2430:TRP:CE3	2.54	0.43
1:B:1774:LEU:HA	1:B:1774:LEU:HD12	1.70	0.43
1:B:2137:VAL:O	1:B:2141:VAL:HG23	2.19	0.43
1:B:2238:LEU:HD23	1:B:2430:TRP:CE3	2.54	0.43
1:B:2244:GLN:OE1	1:B:2244:GLN:N	2.52	0.43
1:B:2276:TYR:CE1	1:B:2449:PHE:HB3	2.53	0.43
1:A:2238:LEU:HD23	1:A:2430:TRP:CE3	2.54	0.42
1:A:2244:GLN:N	1:A:2244:GLN:OE1	2.52	0.42
1:C:1322:LEU:HD22	1:C:1530:MET:HG3	2.00	0.42
1:C:2187:VAL:HG23	2:F:235:ILE:HG12	2.01	0.42
1:C:2238:LEU:HD23	1:C:2430:TRP:CD2	2.54	0.42
1:C:2343:GLU:O	1:C:2344:LEU:HD23	2.19	0.42
1:A:1282:TRP:HA	1:A:1285:ILE:HG22	1.99	0.42
1:A:2352:ARG:HB3	1:A:2352:ARG:CZ	2.48	0.42
1:C:1991:ILE:HD11	1:C:2082:TRP:HE1	1.83	0.42
1:C:2035:ARG:HH12	1:C:2109:PHE:HZ	1.65	0.42
1:C:2070:GLU:OE1	1:C:2075:GLN:HB2	2.19	0.42
1:C:2137:VAL:O	1:C:2141:VAL:HG23	2.19	0.42
1:C:2286:ILE:HG13	1:C:2444:LEU:HB2	2.01	0.42
1:B:1077:ILE:HD11	1:B:1083:PRO:HA	2.01	0.42
1:B:1338:GLU:OE1	1:B:2103:THR:HG22	2.20	0.42
1:B:1552:ARG:HD3	1:B:1553:ARG:HH22	1.83	0.42
1:B:1991:ILE:HD11	1:B:2082:TRP:HE1	1.83	0.42
1:B:2131:LEU:HA	1:B:2131:LEU:HD23	1.69	0.42
1:A:1338:GLU:OE1	1:A:2103:THR:HG22	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1992:ILE:HD13	1:A:1992:ILE:HA	1.89	0.42
1:C:1097:ASP:OD1	1:C:1098:PHE:N	2.52	0.42
1:C:1191:LEU:HA	1:C:1191:LEU:HD23	1.79	0.42
1:C:2338:GLU:CG	1:C:2339:LYS:H	2.32	0.42
1:B:1173:GLY:HA3	1:B:1184:TYR:HB2	2.01	0.42
1:A:1335:ARG:HH22	1:A:1971:ARG:H	1.67	0.42
1:A:2053:LEU:HA	1:A:2053:LEU:HD12	1.81	0.42
1:A:2058:HIS:NE2	1:A:2083:TYR:OH	2.32	0.42
1:A:2133:GLU:CG	1:C:2485:PHE:CD2	3.01	0.42
1:C:2016:VAL:HG12	1:C:2017:PRO:HD3	2.02	0.42
1:B:2070:GLU:OE1	1:B:2075:GLN:HB2	2.19	0.42
1:A:2286:ILE:HG13	1:A:2444:LEU:HB2	2.02	0.42
1:C:1077:ILE:HD11	1:C:1083:PRO:HA	2.01	0.42
1:C:1147:ARG:HD3	1:C:1147:ARG:H	1.84	0.42
1:B:1530:MET:O	1:B:1534:LEU:HD23	2.20	0.42
1:B:2541:LYS:O	1:B:2541:LYS:HG2	2.18	0.42
1:A:1147:ARG:H	1:A:1147:ARG:HD3	1.84	0.42
1:C:1530:MET:O	1:C:1534:LEU:HD23	2.20	0.42
1:B:1147:ARG:H	1:B:1147:ARG:HD3	1.84	0.42
1:B:1334:HIS:HA	1:B:1337:ILE:HG22	2.02	0.42
1:A:1717:TRP:CD1	1:A:1717:TRP:C	2.98	0.42
1:A:2338:GLU:CG	1:A:2339:LYS:H	2.32	0.42
1:A:2485:PHE:HE1	2:D:242:LEU:HD11	1.84	0.42
1:C:970:LEU:HD12	1:C:977:CYS:HA	2.01	0.42
1:C:1717:TRP:CD1	1:C:1717:TRP:C	2.98	0.42
1:C:2047:LEU:HA	1:C:2097:ILE:HD13	2.02	0.42
1:C:2541:LYS:O	1:C:2541:LYS:HG2	2.18	0.42
1:B:2128:VAL:CG1	1:B:2131:LEU:HD12	2.49	0.42
1:A:1020:ILE:HG23	1:A:1033:TRP:CH2	2.55	0.42
1:C:1020:ILE:HG23	1:C:1033:TRP:CH2	2.55	0.42
1:C:2121:LEU:HD23	1:C:2121:LEU:HA	1.77	0.42
1:B:1992:ILE:HD13	1:B:1992:ILE:HA	1.89	0.42
1:B:2380:ASN:OD1	1:B:2453:VAL:HG22	2.19	0.42
1:A:1540:LEU:HA	1:A:1543:GLN:HG2	2.01	0.42
1:A:2016:VAL:HG12	1:A:2017:PRO:HD3	2.02	0.42
1:A:2070:GLU:OE1	1:A:2075:GLN:HB2	2.19	0.42
1:A:2380:ASN:OD1	1:A:2453:VAL:HG22	2.19	0.42
1:C:1173:GLY:HA3	1:C:1184:TYR:HB2	2.01	0.42
1:C:1326:ALA:N	1:C:1649:LEU:HD21	2.35	0.42
1:C:1553:ARG:HH11	1:C:1556:LEU:HD11	1.85	0.42
1:C:2405:LEU:HD12	1:C:2430:TRP:CE2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1335:ARG:HH22	1:B:1971:ARG:H	1.67	0.42
1:B:2343:GLU:O	1:B:2344:LEU:HD23	2.19	0.42
1:A:2492:ILE:HD13	1:A:2492:ILE:HG21	1.85	0.42
1:C:1996:TRP:CZ3	1:B:2467:VAL:HG13	2.55	0.42
1:C:2361:ARG:HH11	1:C:2364:GLN:CD	2.27	0.42
1:B:1200:GLN:H	1:B:1200:GLN:HG2	1.72	0.42
1:B:1694:ILE:HD13	1:B:1694:ILE:HA	1.88	0.42
1:B:2016:VAL:HG12	1:B:2017:PRO:HD3	2.02	0.42
1:A:970:LEU:HD12	1:A:977:CYS:HA	2.01	0.41
1:A:1081:TYR:O	1:A:1082:LEU:HD22	2.20	0.41
1:A:2221:ASN:HB2	1:A:2453:VAL:HG23	2.02	0.41
1:A:2485:PHE:CD1	1:B:2153:MET:HE2	2.54	0.41
1:C:988:LYS:HD3	1:C:988:LYS:HA	1.76	0.41
1:B:1020:ILE:HG23	1:B:1033:TRP:CH2	2.55	0.41
1:B:2047:LEU:HA	1:B:2097:ILE:HD13	2.02	0.41
1:B:2221:ASN:HB2	1:B:2453:VAL:HG23	2.02	0.41
1:A:1047:GLN:HA	1:A:1050:LEU:HB2	2.02	0.41
1:A:1077:ILE:HD11	1:A:1083:PRO:HA	2.01	0.41
1:C:1338:GLU:OE1	1:C:2103:THR:HG22	2.19	0.41
1:B:1090:ASN:OD1	1:B:1091:SER:N	2.54	0.41
1:B:1553:ARG:HH11	1:B:1556:LEU:HD11	1.85	0.41
1:A:1090:ASN:OD1	1:A:1091:SER:N	2.53	0.41
1:A:1204:ARG:HD2	1:A:1204:ARG:HA	1.88	0.41
1:A:2204:TRP:CZ2	1:B:2025:LEU:HD12	2.55	0.41
1:A:2207:LEU:HD12	1:A:2207:LEU:HA	1.78	0.41
1:A:2354:LEU:HD23	1:A:2354:LEU:HA	1.91	0.41
1:C:2089:TYR:CD2	1:C:2089:TYR:C	2.98	0.41
1:B:1540:LEU:HA	1:B:1543:GLN:HG2	2.01	0.41
1:B:2467:VAL:O	1:B:2471:VAL:HG12	2.20	0.41
1:A:1326:ALA:N	1:A:1649:LEU:HD21	2.35	0.41
1:A:2405:LEU:HD12	1:A:2430:TRP:CE2	2.55	0.41
1:A:2429:TRP:HZ2	1:C:2299:PRO:HG2	1.85	0.41
1:C:1207:LEU:HD13	1:C:1207:LEU:HA	1.91	0.41
1:B:1047:GLN:HA	1:B:1050:LEU:HB2	2.02	0.41
1:B:1326:ALA:N	1:B:1649:LEU:HD21	2.35	0.41
1:B:1783:ILE:HG13	1:B:1783:ILE:O	2.21	0.41
1:B:2089:TYR:CD2	1:B:2089:TYR:C	2.98	0.41
1:B:2349:THR:HA	1:B:2352:ARG:NH2	2.35	0.41
1:B:2443:LEU:HA	1:B:2443:LEU:HD23	1.82	0.41
1:B:2492:ILE:HG21	1:B:2492:ILE:HD13	1.85	0.41
1:A:1173:GLY:HA3	1:A:1184:TYR:HB2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1185:LEU:HD23	1:A:1185:LEU:HA	1.73	0.41
1:A:1281:ILE:HG23	1:A:1282:TRP:N	2.36	0.41
1:C:1744:LYS:NZ	1:C:1775:GLY:O	2.52	0.41
1:C:1984:ASP:CB	1:C:2031:MET:HE2	2.46	0.41
1:B:1717:TRP:CD1	1:B:1717:TRP:C	2.98	0.41
1:B:2191:MET:HE1	2:E:239:CYS:N	2.35	0.41
1:B:2338:GLU:CG	1:B:2339:LYS:H	2.32	0.41
1:A:1149:TYR:HD1	1:A:1665:PHE:HZ	1.68	0.41
1:A:1334:HIS:HA	1:A:1337:ILE:HG22	2.02	0.41
1:A:1553:ARG:HH11	1:A:1556:LEU:HD11	1.85	0.41
1:A:2121:LEU:HD23	1:A:2121:LEU:HA	1.77	0.41
1:C:1515:GLY:O	1:C:1518:ARG:HG2	2.21	0.41
1:A:1985:ILE:HD13	1:A:1985:ILE:HA	1.92	0.41
1:A:2028:PHE:HB3	1:C:2200:ILE:HD13	2.03	0.41
1:C:1281:ILE:HG23	1:C:1282:TRP:N	2.36	0.41
1:B:1744:LYS:NZ	1:B:1775:GLY:O	2.52	0.41
1:B:2092:LEU:HD23	1:B:2092:LEU:HA	1.76	0.41
1:C:2207:LEU:HD12	1:C:2207:LEU:HA	1.77	0.41
1:C:2467:VAL:O	1:C:2471:VAL:HG12	2.20	0.41
1:C:2519:LEU:HA	1:C:2519:LEU:HD23	1.76	0.41
1:B:1281:ILE:HG23	1:B:1282:TRP:N	2.36	0.41
1:B:2405:LEU:HD12	1:B:2430:TRP:CE2	2.55	0.41
1:A:1530:MET:O	1:A:1534:LEU:HD23	2.20	0.41
1:A:1552:ARG:HG2	1:A:1553:ARG:NH1	2.36	0.41
1:A:2089:TYR:CD2	1:A:2089:TYR:C	2.98	0.41
1:A:2467:VAL:O	1:A:2471:VAL:HG12	2.20	0.41
1:C:1013:HIS:CD2	1:C:1047:GLN:HE22	2.39	0.41
1:C:1090:ASN:OD1	1:C:1091:SER:N	2.53	0.41
1:C:1773:ILE:HD13	1:C:1773:ILE:HA	1.88	0.41
1:C:1800:LEU:HD22	1:C:1806:TRP:CE3	2.56	0.41
1:C:2015:GLN:HB3	1:C:2016:VAL:H	1.71	0.41
1:C:2128:VAL:CG1	1:C:2131:LEU:HD12	2.49	0.41
1:C:2371:LEU:N	1:C:2399:LEU:O	2.47	0.41
1:B:1033:TRP:HA	1:B:1036:TYR:HB3	2.03	0.41
1:B:2165:ILE:HG23	1:B:2165:ILE:HD12	1.78	0.41
1:A:1189:PHE:CZ	1:A:1741:VAL:HG11	2.55	0.41
1:A:2188:LYS:HG2	1:B:2140:TRP:CZ2	2.56	0.41
1:C:1017:LEU:HA	1:C:1020:ILE:HD12	2.03	0.41
1:C:1081:TYR:O	1:C:1082:LEU:HD22	2.21	0.41
1:C:2041:LYS:CG	1:C:2105:ILE:HD13	2.51	0.41
1:B:2015:GLN:HB3	1:B:2016:VAL:H	1.71	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2059:ILE:HD13	1:B:2059:ILE:HA	1.90	0.41
1:A:1017:LEU:HA	1:A:1020:ILE:HD12	2.03	0.40
1:A:1024:ARG:HB2	1:A:1294:ARG:HH22	1.86	0.40
1:A:1200:GLN:H	1:A:1200:GLN:HG2	1.72	0.40
1:A:1701:VAL:HG12	1:A:1702:THR:N	2.36	0.40
1:A:2258:GLU:O	1:A:2261:GLN:HG2	2.21	0.40
1:C:1515:GLY:HA2	1:C:1518:ARG:HG2	2.03	0.40
1:C:1552:ARG:HG2	1:C:1553:ARG:NH1	2.36	0.40
1:C:2221:ASN:HB2	1:C:2453:VAL:HG23	2.02	0.40
1:C:2245:GLN:HG2	1:B:2339:LYS:NZ	2.36	0.40
1:C:2280:ASP:O	1:C:2450:SER:OG	2.37	0.40
1:C:2349:THR:HA	1:C:2352:ARG:NH2	2.35	0.40
1:B:1081:TYR:O	1:B:1082:LEU:HD22	2.20	0.40
1:B:1515:GLY:O	1:B:1518:ARG:HG2	2.21	0.40
1:B:2191:MET:HE1	2:E:238:GLU:C	2.46	0.40
1:B:2280:ASP:O	1:B:2450:SER:OG	2.37	0.40
1:B:2475:LEU:HD23	1:B:2475:LEU:HA	1.83	0.40
1:A:1800:LEU:HD22	1:A:1806:TRP:CE3	2.56	0.40
1:A:2092:LEU:HD23	1:A:2092:LEU:HA	1.76	0.40
1:C:1016:TRP:CE2	1:C:1043:PHE:HE2	2.39	0.40
1:C:1047:GLN:HA	1:C:1050:LEU:HB2	2.02	0.40
1:C:1358:LYS:HB2	1:C:1358:LYS:HE3	1.93	0.40
1:C:1701:VAL:HG12	1:C:1702:THR:N	2.36	0.40
1:C:2149:LEU:HA	1:C:2149:LEU:HD12	1.70	0.40
1:B:1115:ARG:O	1:B:1117:GLU:N	2.55	0.40
1:B:1552:ARG:HG2	1:B:1553:ARG:NH1	2.36	0.40
1:B:2258:GLU:O	1:B:2261:GLN:HG2	2.21	0.40
1:B:2286:ILE:HG13	1:B:2444:LEU:HB2	2.01	0.40
1:B:2422:LYS:HD3	1:B:2422:LYS:HA	1.93	0.40
1:A:2324:GLN:HB2	1:A:2335:TYR:HE2	1.86	0.40
1:A:2485:PHE:CG	1:B:2153:MET:CE	3.05	0.40
1:A:2525:LEU:HA	1:A:2525:LEU:HD23	1.76	0.40
1:C:1149:TYR:HD1	1:C:1665:PHE:HZ	1.68	0.40
1:C:1992:ILE:HD13	1:C:1992:ILE:HA	1.89	0.40
1:C:2308:LEU:HA	1:C:2351:ARG:HD3	2.03	0.40
1:B:1016:TRP:CE2	1:B:1043:PHE:HE2	2.39	0.40
1:B:1185:LEU:HA	1:B:1185:LEU:HD23	1.73	0.40
1:B:1701:VAL:HG12	1:B:1702:THR:N	2.36	0.40
1:B:1800:LEU:HD22	1:B:1806:TRP:CE3	2.56	0.40
1:B:2121:LEU:HD23	1:B:2121:LEU:HA	1.77	0.40
1:A:1016:TRP:CE2	1:A:1043:PHE:HE2	2.38	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1033:TRP:HA	1:A:1036:TYR:HB3	2.03	0.40
1:A:1515:GLY:O	1:A:1518:ARG:HG2	2.21	0.40
1:A:1528:ARG:O	1:A:1531:SER:OG	2.33	0.40
1:A:1716:LEU:HA	1:A:1716:LEU:HD23	1.63	0.40
1:A:2108:ASN:HB3	1:A:2111:THR:CG2	2.47	0.40
1:A:2323:PHE:CE1	1:A:2448:ILE:HG21	2.57	0.40
1:A:2376:ILE:HB	1:A:2448:ILE:HG22	2.04	0.40
1:C:1033:TRP:HA	1:C:1036:TYR:HB3	2.03	0.40
1:C:1328:LEU:HD23	1:C:1328:LEU:HA	1.85	0.40
1:C:1717:TRP:CD1	1:C:1717:TRP:O	2.75	0.40
1:C:1783:ILE:HG13	1:C:1783:ILE:O	2.21	0.40
1:C:2258:GLU:O	1:C:2261:GLN:HG2	2.21	0.40
1:C:2324:GLN:HB2	1:C:2335:TYR:HE2	1.86	0.40
1:B:1017:LEU:HA	1:B:1020:ILE:HD12	2.03	0.40
1:B:2308:LEU:HA	1:B:2351:ARG:HD3	2.04	0.40
1:A:1203:THR:HA	1:A:1206:GLN:NE2	2.37	0.40
1:A:2308:LEU:HA	1:A:2351:ARG:HD3	2.04	0.40
1:A:2372:PHE:CD2	1:A:2434:LEU:HD21	2.53	0.40
1:C:1334:HIS:HA	1:C:1337:ILE:HG22	2.02	0.40
1:C:2033:ILE:HD13	1:C:2033:ILE:HA	1.91	0.40
1:B:1717:TRP:CD1	1:B:1717:TRP:O	2.75	0.40
1:B:2371:LEU:N	1:B:2399:LEU:O	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1193/2815 (42%)	1098 (92%)	95 (8%)	0	100	100
1	B	1193/2815 (42%)	1097 (92%)	96 (8%)	0	100	100
1	C	1193/2815 (42%)	1098 (92%)	95 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	19/269 (7%)	18 (95%)	1 (5%)	0	100	100
2	E	19/269 (7%)	18 (95%)	1 (5%)	0	100	100
2	F	19/269 (7%)	18 (95%)	1 (5%)	0	100	100
All	All	3636/9252 (39%)	3347 (92%)	289 (8%)	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	983/2477 (40%)	983 (100%)	0	100	100
1	B	983/2477 (40%)	983 (100%)	0	100	100
1	C	983/2477 (40%)	983 (100%)	0	100	100
2	D	19/218 (9%)	19 (100%)	0	100	100
2	E	19/218 (9%)	19 (100%)	0	100	100
2	F	19/218 (9%)	19 (100%)	0	100	100
All	All	3006/8085 (37%)	3006 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1047	GLN
1	A	1225	ASN
1	A	1408	HIS
1	A	1526	HIS
1	A	1543	GLN
1	A	1698	ASN
1	A	1748	GLN
1	A	2389	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1047	GLN
1	C	1225	ASN
1	C	1408	HIS
1	C	1526	HIS
1	C	1543	GLN
1	C	1698	ASN
1	C	1748	GLN
1	C	2389	GLN
1	C	2490	HIS
1	B	1047	GLN
1	B	1225	ASN
1	B	1526	HIS
1	B	1543	GLN
1	B	1698	ASN
1	B	1748	GLN
1	B	2244	GLN
1	B	2389	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

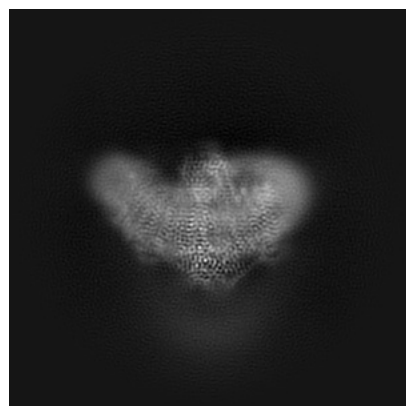
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64998. These allow visual inspection of the internal detail of the map and identification of artifacts.

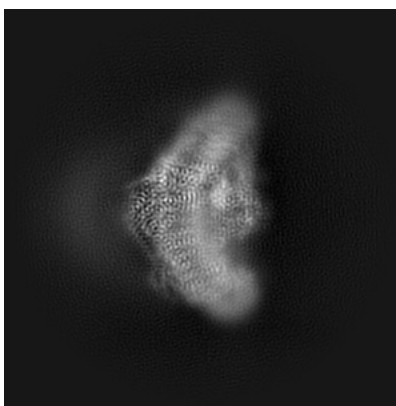
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

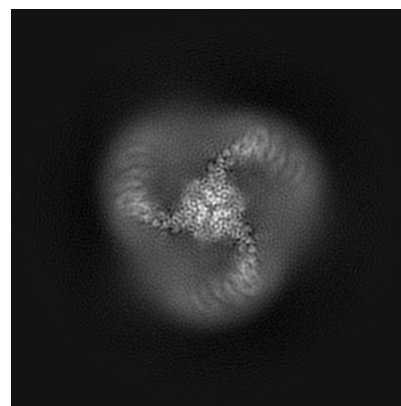
6.1.1 Primary map



X

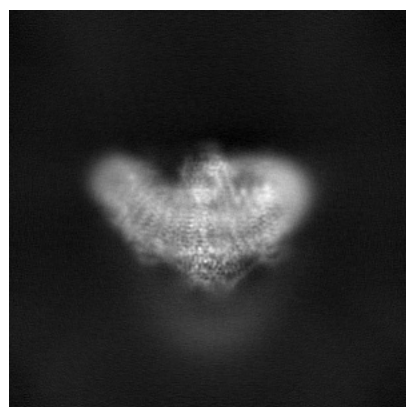


Y

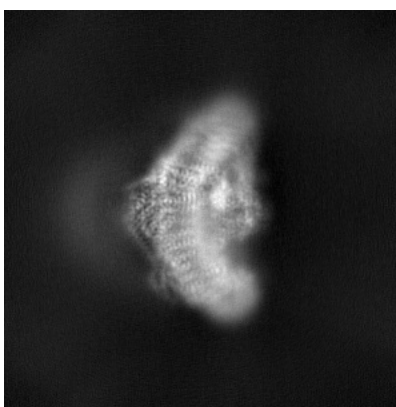


Z

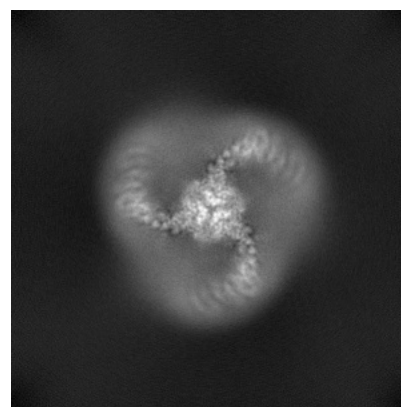
6.1.2 Raw map



X



Y

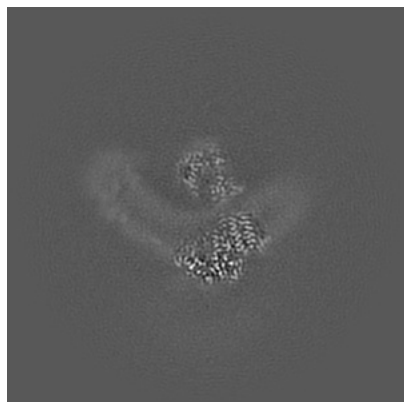


Z

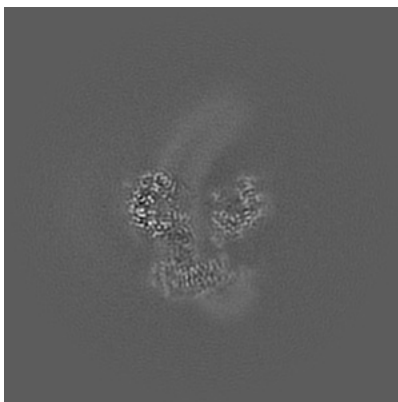
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

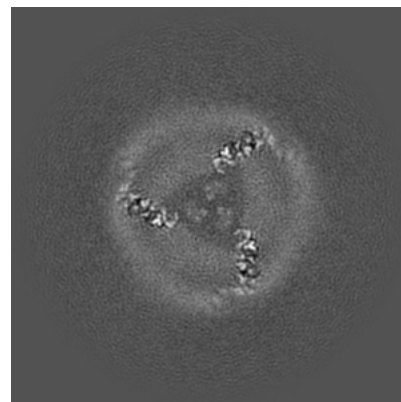
6.2.1 Primary map



X Index: 190

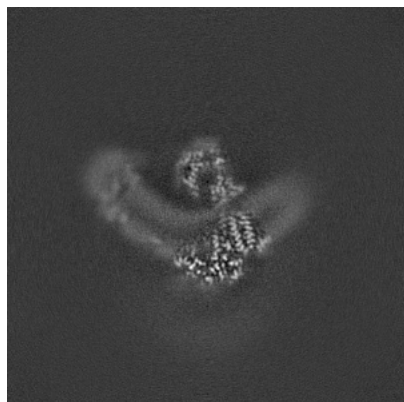


Y Index: 190

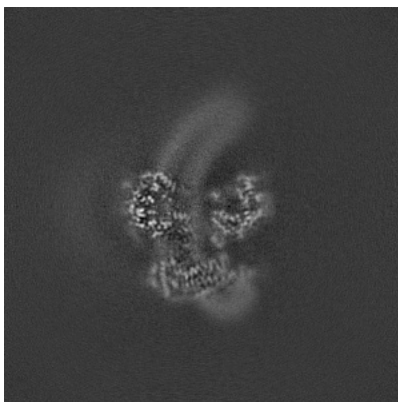


Z Index: 190

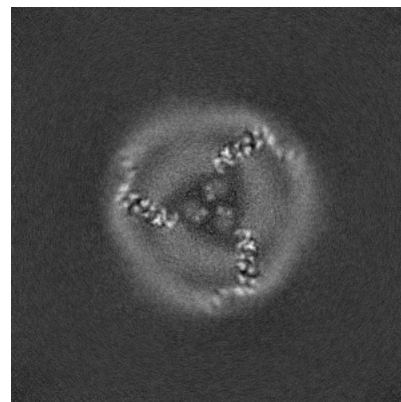
6.2.2 Raw map



X Index: 190



Y Index: 190

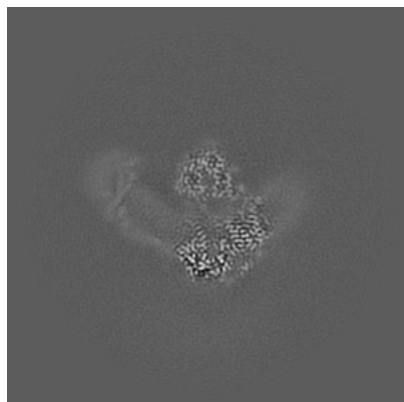


Z Index: 190

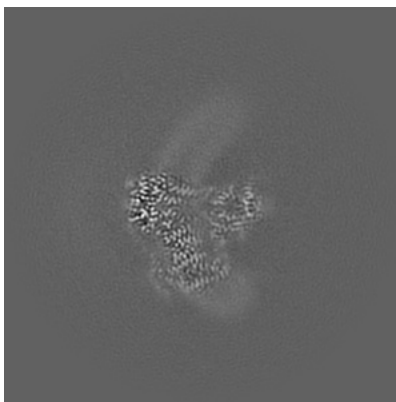
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

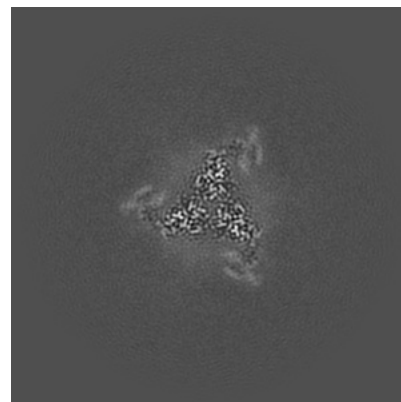
6.3.1 Primary map



X Index: 198

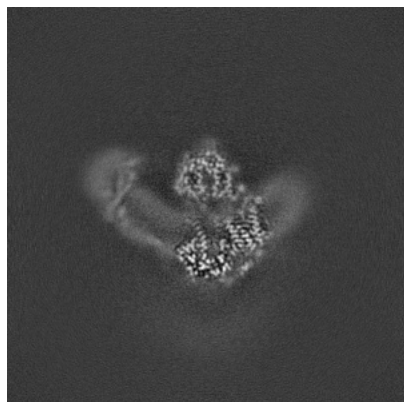


Y Index: 185

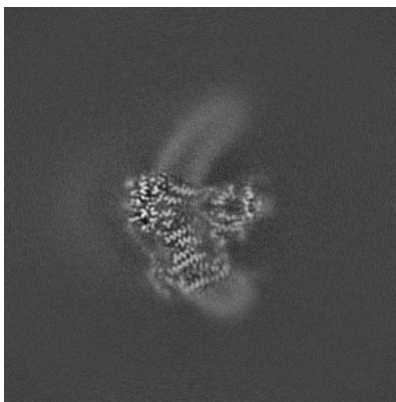


Z Index: 153

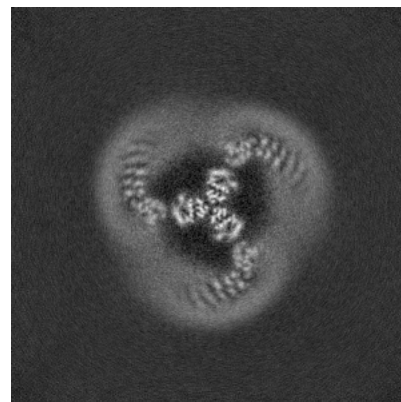
6.3.2 Raw map



X Index: 198



Y Index: 185

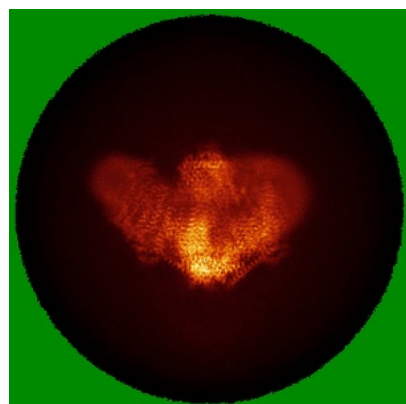


Z Index: 208

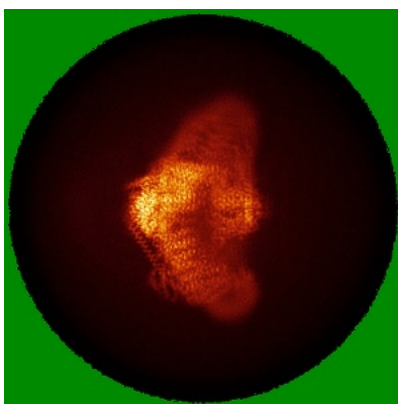
The images above show the largest variance slices of the map in three orthogonal directions.

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

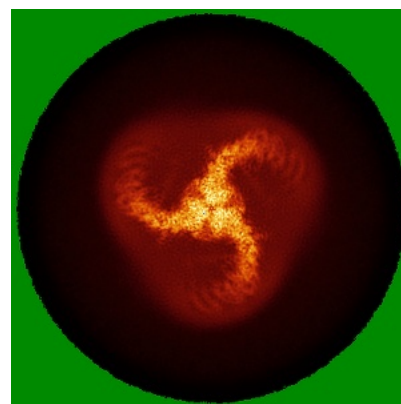
6.4.1 Primary map



X

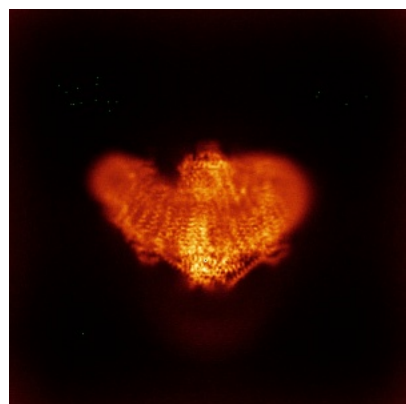


Y

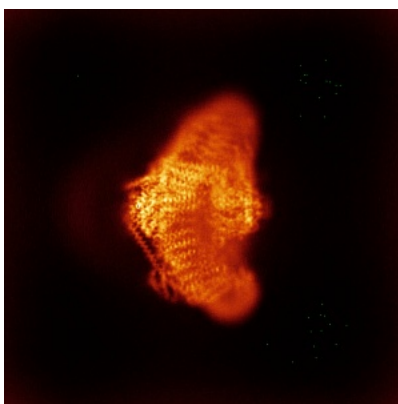


Z

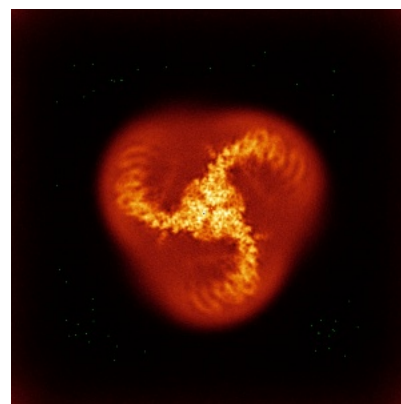
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.34. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

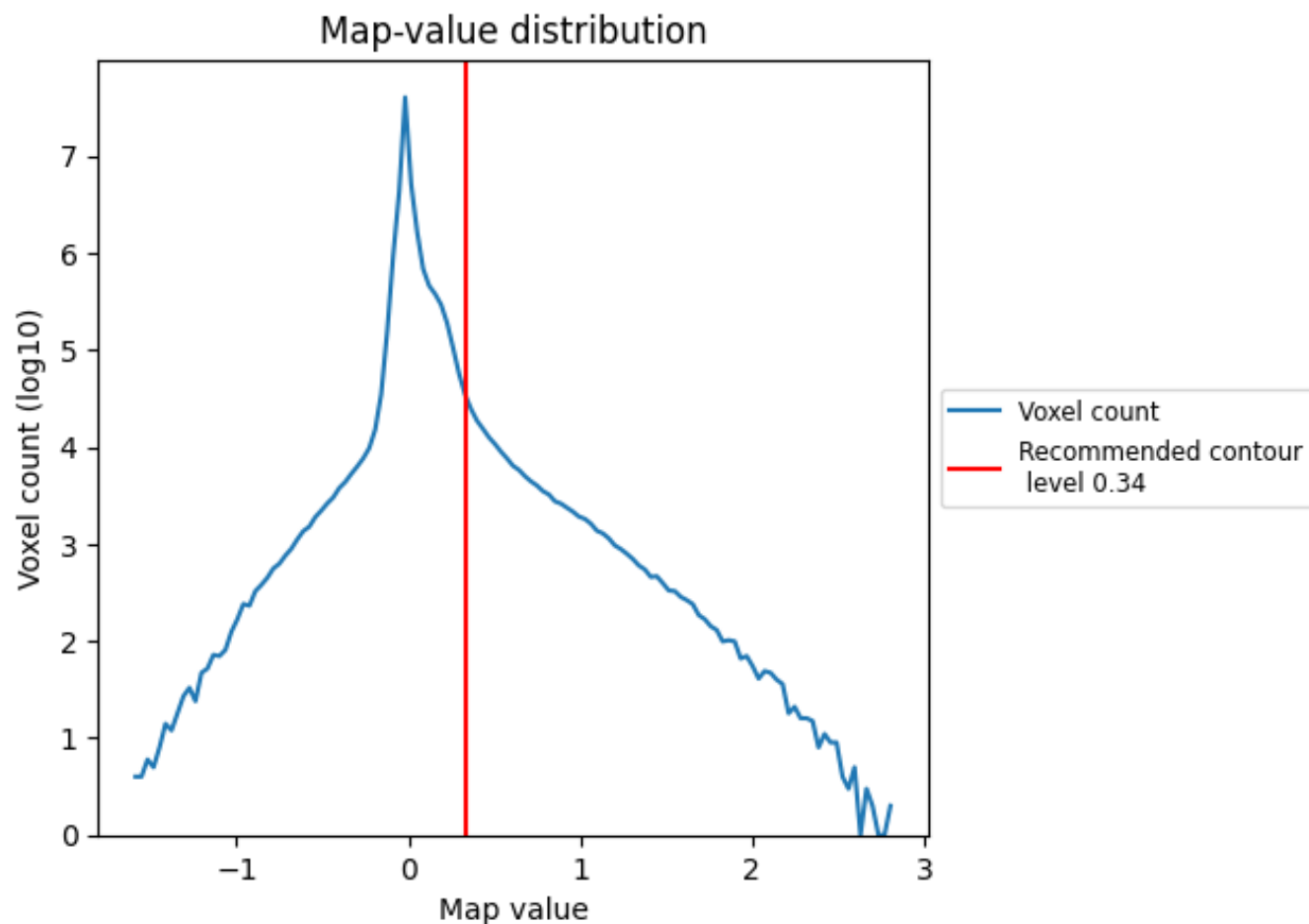
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

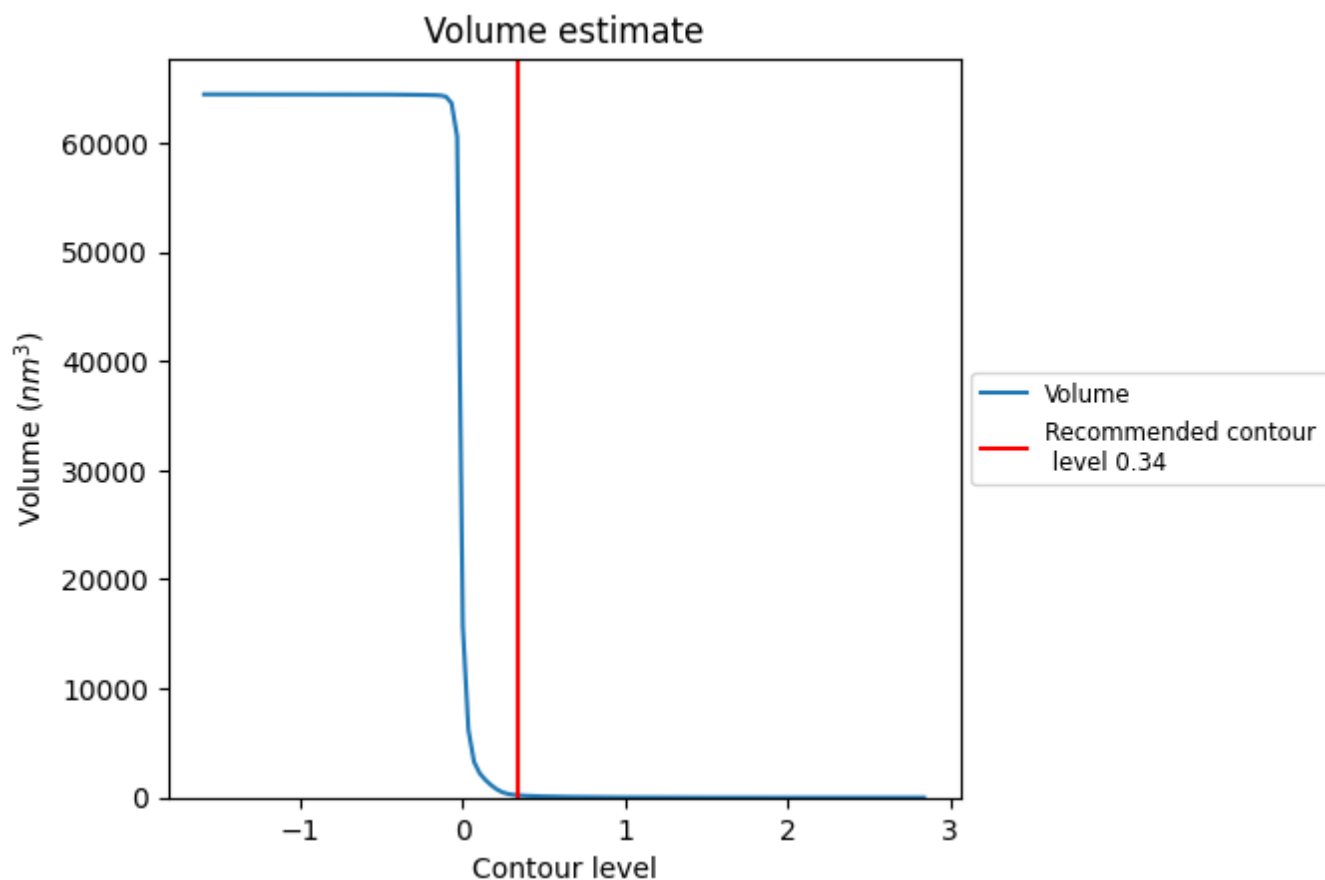
This section contains the results of statistical analysis of the map.

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.

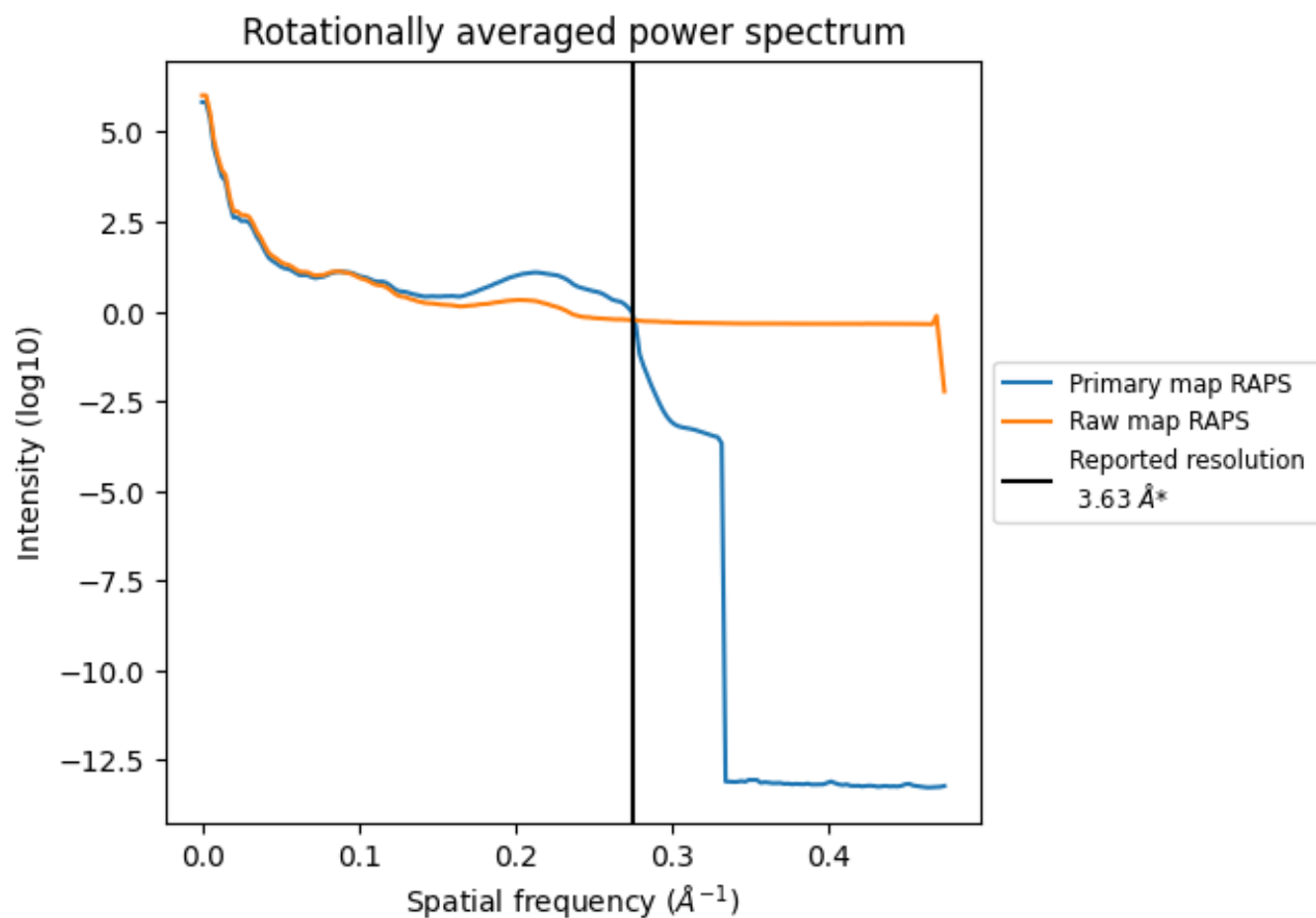
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 215 nm³; this corresponds to an approximate mass of 194 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 ⓘ

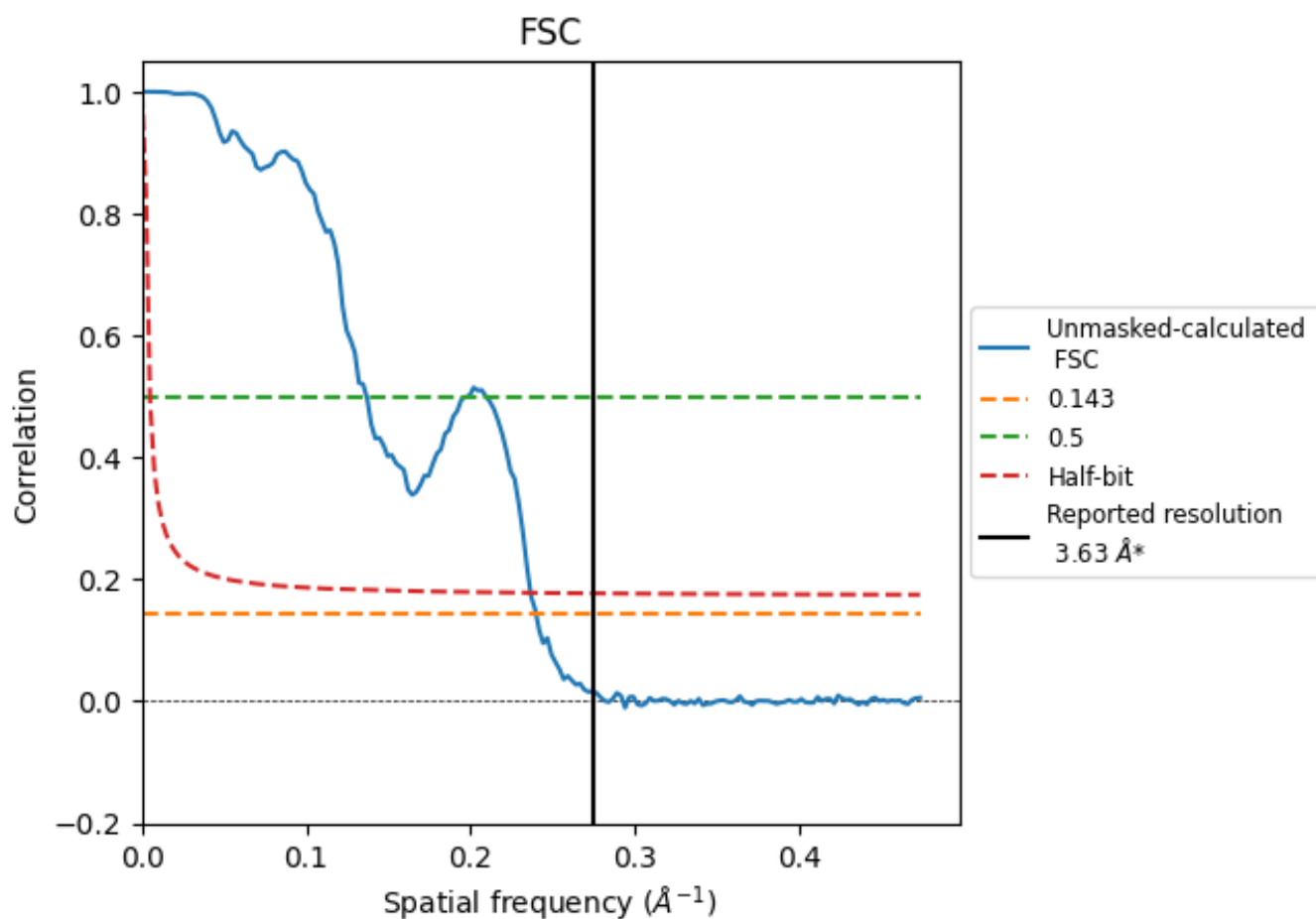


*Reported resolution corresponds to spatial frequency of 0.275 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.275 \AA^{-1}

8.2 Resolution estimates [i](#)

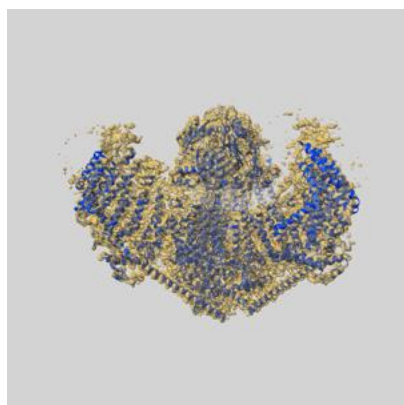
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.63	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.17	7.31	4.22

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.17 differs from the reported value 3.63 by more than 10 %

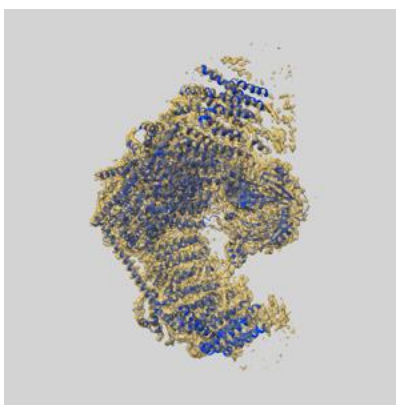
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-64998 and PDB model 9VED. Per-residue inclusion information can be found in section [3](#) on page [9](#).

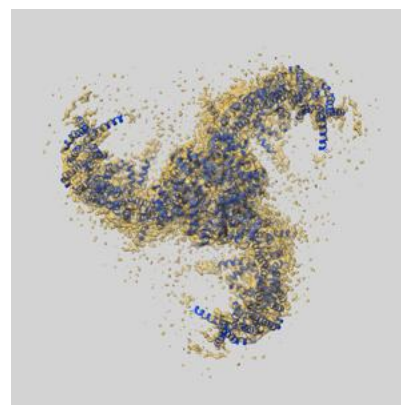
9.1 Map-model overlay [i](#)



X



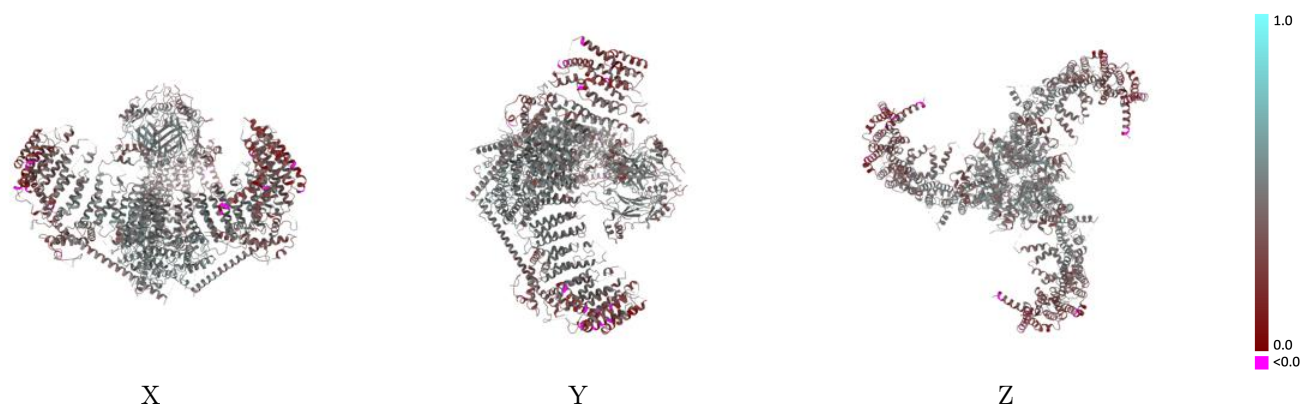
Y



Z

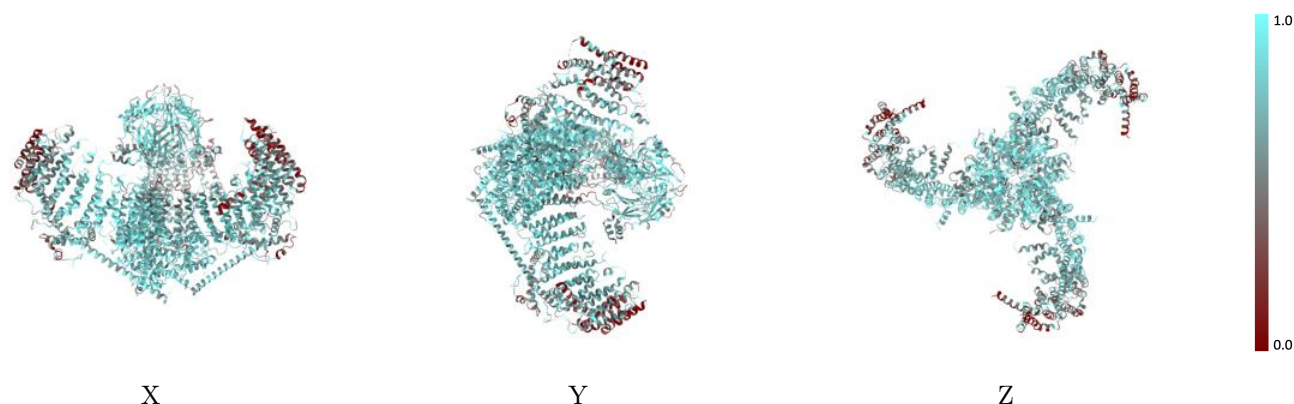
The images above show the 3D surface view of the map at the recommended contour level 0.34 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



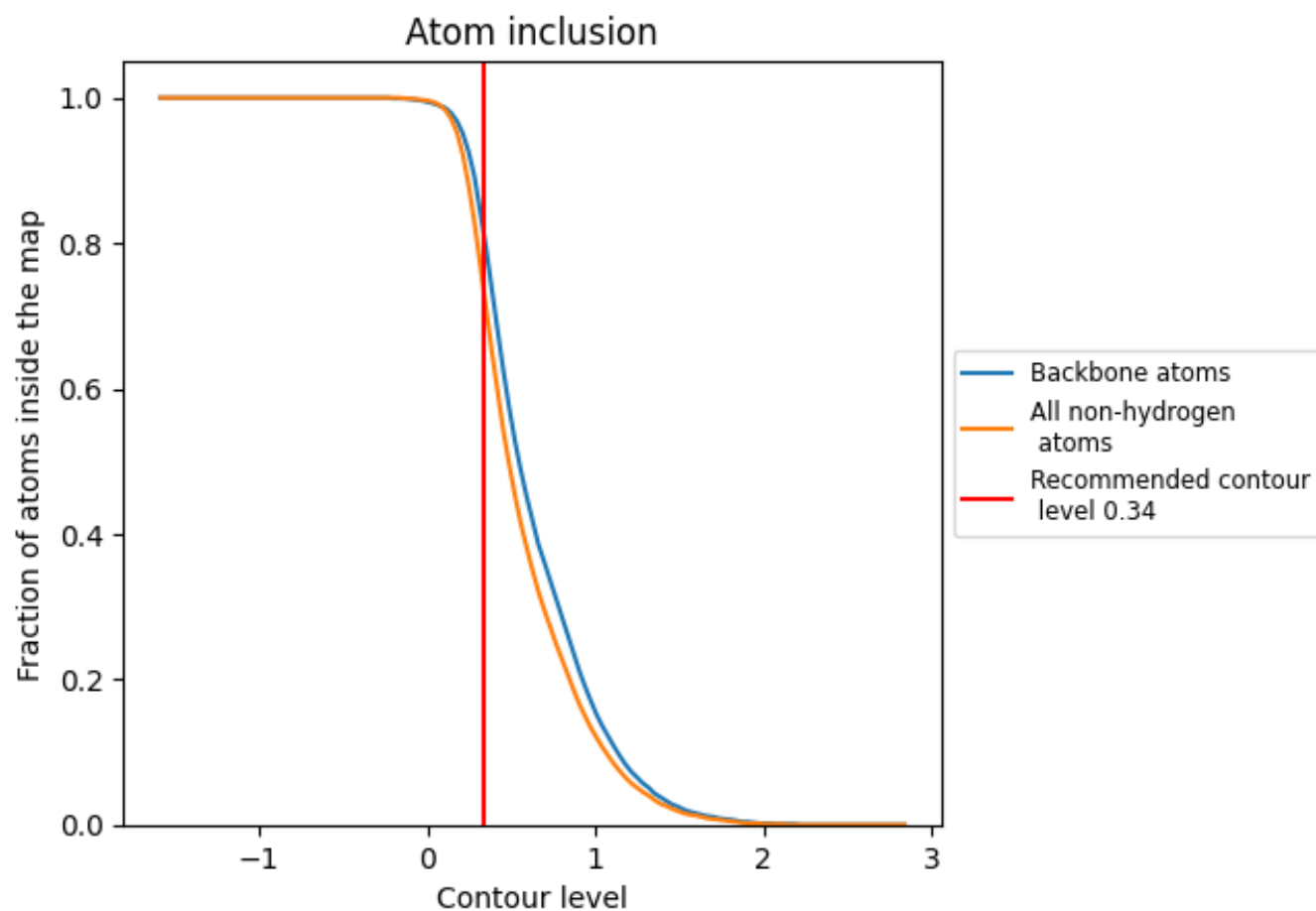
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.34).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.34) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7280	<div><div></div></div> 0.4340
A	<div><div></div></div> 0.7260	<div><div></div></div> 0.4290
B	<div><div></div></div> 0.7300	<div><div></div></div> 0.4360
C	<div><div></div></div> 0.7280	<div><div></div></div> 0.4350
D	<div><div></div></div> 0.6960	<div><div></div></div> 0.4690
E	<div><div></div></div> 0.6820	<div><div></div></div> 0.4710
F	<div><div></div></div> 0.7030	<div><div></div></div> 0.4780

1.0

0.0

<0.0