



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:14 PM UTC

PDB ID : 6KG7 / pdb_00006kg7
EMDB ID : EMD-9975
Title : Cryo-EM Structure of the Mammalian Tactile Channel Piezo2
Authors : Wang, L.; Zhou, H.; Zhang, M.; Liu, W.; Deng, T.; Zhao, Q.; Li, Y.; Lei, J.;
Li, X.; Xiao, B.
Deposited on : 2019-07-11
Resolution : 3.80 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
Mogul : 2022.3.0, CSD as543be (2022)
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

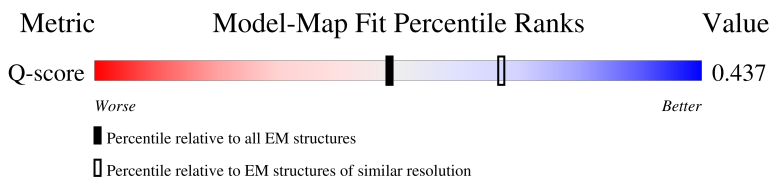
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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	2822	 50% 14% 36%
1	B	2822	 50% 14% 36%
1	C	2822	 50% 15% 36%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 44892 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 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1817	Total	C	N	O	S	1	0
			14908	9922	2377	2508	101		
1	B	1817	Total	C	N	O	S	1	0
			14908	9922	2377	2508	101		
1	C	1817	Total	C	N	O	S	1	0
			14908	9922	2377	2508	101		

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	

Continued on next page...

Continued from previous page...

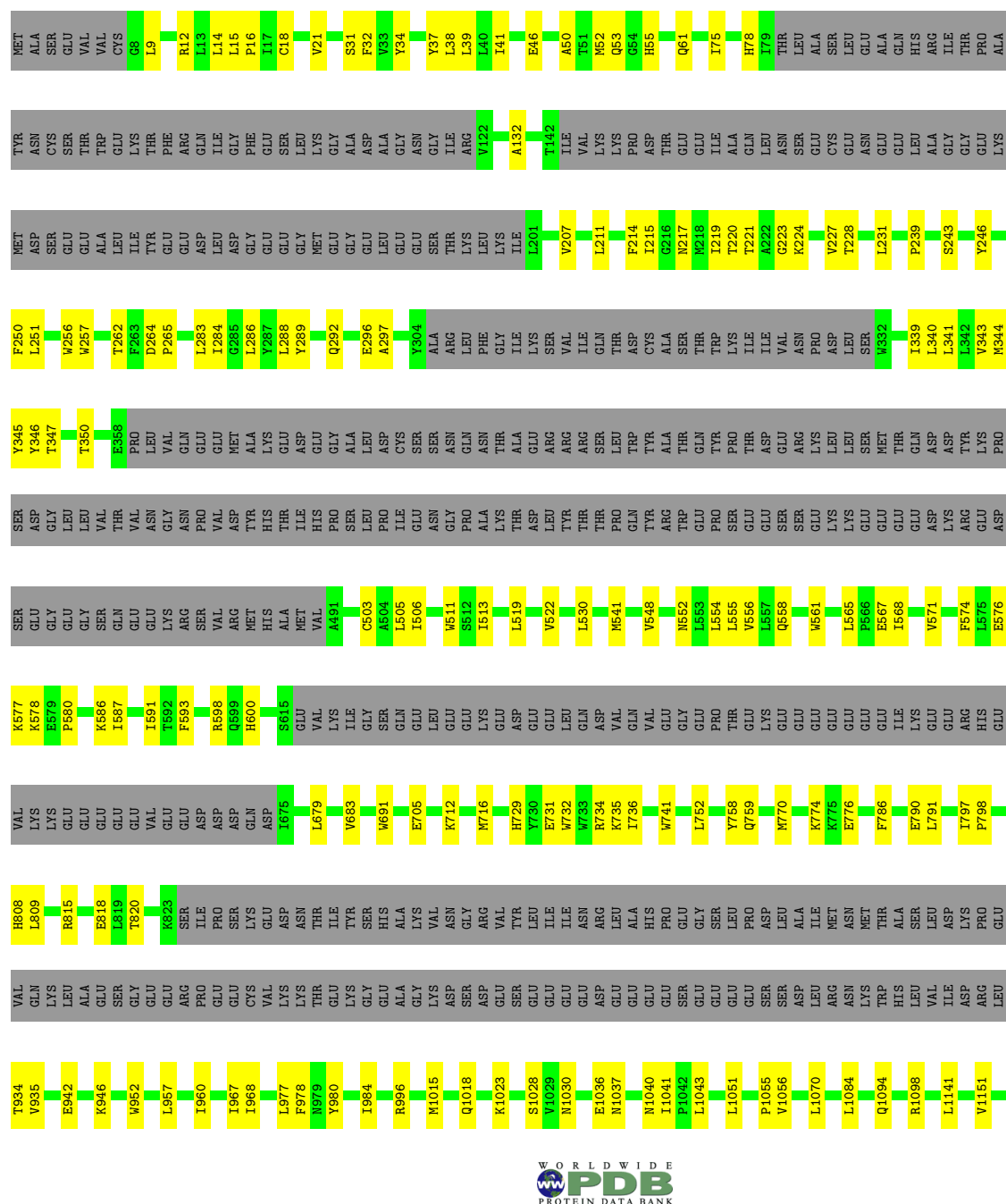
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	



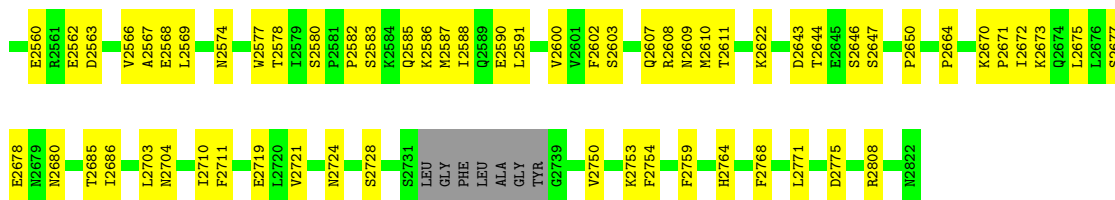


● Molecule 1: Piezo-type mechanosensitive ion channel component 2

Chain B: 50% 14% 36%

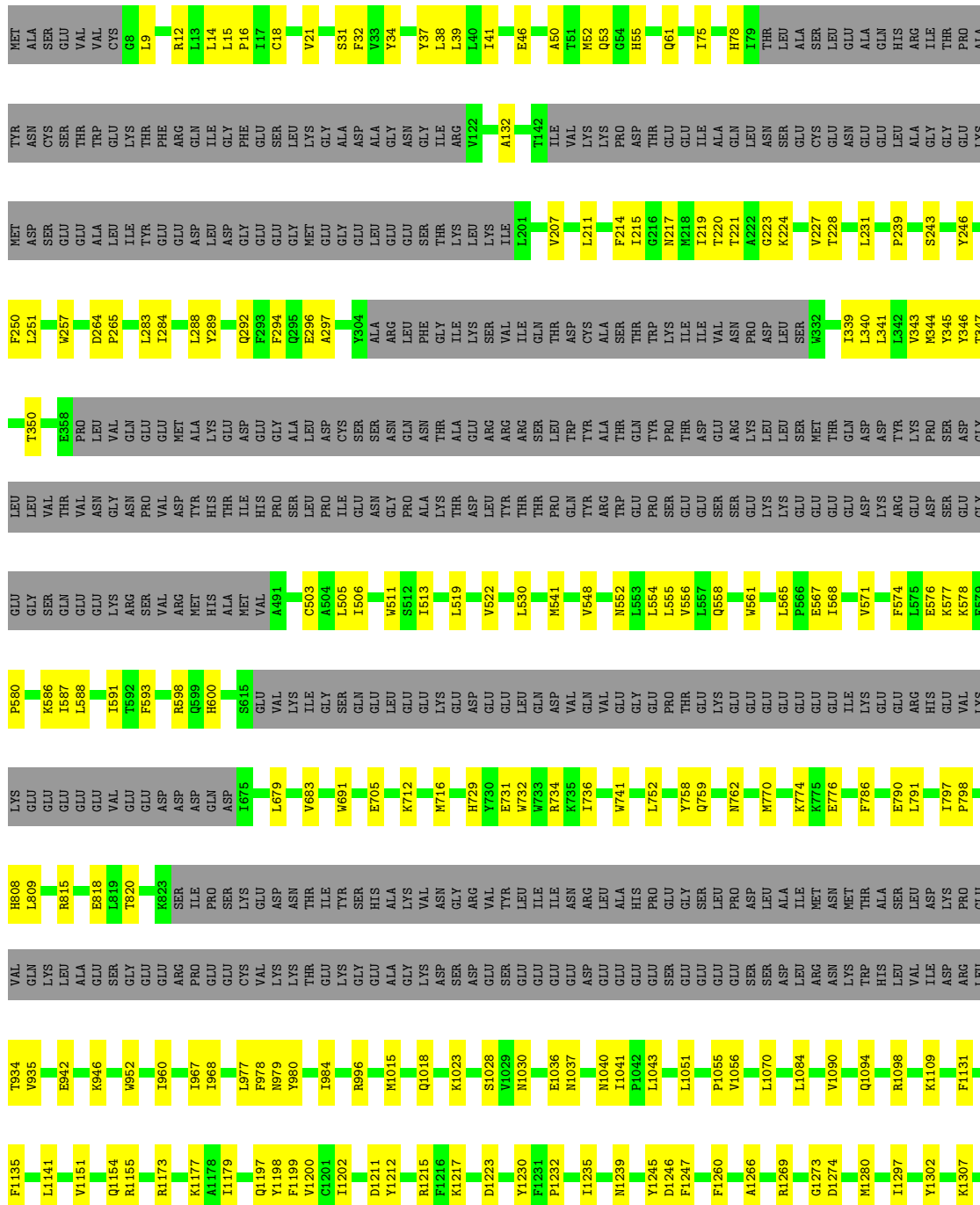


L2491	Q2310	GLU	VAL	ILE	M1955	SER	LEU	GLU	R1707	ARG	TRP	GLY	I1330	Q1154
F2492	T2313	LEU	HIS	THR	M1956	THR	TYR	TYR	E1708	ARG	GLY	GLU	F1333	R1156
MET	T2316	TYR	VAL	LYS	K1957	ASP	GLU	THR	I1709	GLY	ASP	LYS	D1157	D1157
SER	V2316	MET	THR	GLU	M1958	ASP	ARG	GLN	G1712	SER	R1563	GLY	C1341	F1158
ILE	V2316	GLU	PHE	ARG	F1959	CYS	GLN	GLY	G1712	GLY	R1564	GLY	Y1159	Y1159
LYS	V2330	LYS	PRO	THR	H1960	ALA	THR	THR	T1716	ASP	D1574	C1435	L1351	H1163
GLN	V2337	GLN	GLU	PHE	D1961	PRO	THR	THR	R1717	GLY	E1577	L1439	I1356	R1173
VAL	V2337	PRO	PRO	PRO	D1962	SER	GLN	GLN	S1719	VAL	GLU	PRO	W1363	I1179
ALA	I2340	ALA	ALA	TYR	L1964	THR	ILE	THR	I1720	GLU	GLU	D1457	W1363	Q1197
G2501	I2340	ILE	ILE	N2075	E1968	SER	GLU	LEU	H1721	THR	GLU	Q1473	L1366	Y1198
♦	W2344	LYS	ARG	K2082	K1969	LYS	GLU	ASP	M1722	TRP	GLU	Y1477	I1367	F1199
N2504	I2348	ALA	ARG	L2090	F1970	ALA	VAL	ASP	Y1724	ASP	GLU	R1483	A1368	V1200
Q2505	L2348	LYS	LYS	L2090	Y1971	SER	ALA	LEU	I1725	ARG	LYS	Y1477	Y1369	C1201
L2507	E2353	ALA	ARG	H2099	V1972	SER	GLU	GLY	I1727	GLU	ASP	R1483	I1382	I1202
D2508	E2353	THR	CYS	H2099	V1972	PHE	GLU	GLN	ILE	GLU	ASP	R1483	GLY	I1202
V2509	L2364	THR	VAL	E2111	Y1982	HIS	GLU	ASP	ILE	PRO	GLU	R1483	ALA	D1211
♦	W2365	ILE	SER	E2111	Y1982	LEU	GLU	PRO	MET	VAL	GLU	R1483	ALA	Y1212
I2513	W2365	LYS	SER	ASP	M1986	SER	GLU	VAL	ASN	VAL	GLU	R1483	ALA	R1215
T2514	V2368	LYS	SER	ASP	T1987	THR	GLU	VAL	ASN	VAL	GLU	R1483	ALA	F1216
L2515	W2368	THR	ILE	ILE	T1987	PHE	VAL	PRO	SER	THR	GLU	R1483	ALA	K1217
G2516	K2369	LEU	ILE	VAL	L1988	ALA	VAL	LYS	ARG	GLY	THR	R1483	ALA	D1223
C2517	C2370	Q2236	SER	ASP	V1989	SER	GLY	THR	GLU	THR	GLU	R1483	ALA	W1228
Y2518	Q2379	I2237	PRO	SER	A1990	GLN	GLY	GLY	SER	ASP	LYS	R1483	ALA	L1229
Q2519	I2380	I2237	ARG	ASN	R1991	ASP	LEU	GLU	GLY	ASP	THR	R1483	ALA	Y1230
Y2520	I2380	V2256	SER	THR	S1992	ASP	LEU	ARG	GLU	GLU	GLY	R1483	ALA	F1232
I2521	G2383	V2261	SER	THR	E1993	SER	PRO	ALA	ASP	THR	GLY	R1483	ALA	P1232
♦	W2391	L2262	PHE	LYS	M1994	GLY	LEU	PRO	ILE	ILE	THR	R1483	ALA	I1235
M2524	N2391	D2270	SER	GLY	V1995	ALA	HIS	ARG	ASP	ASP	VAL	R1483	ALA	W1239
S2525	T2394	F2271	ASN	GLY	C1996	LYS	GLY	THR	GLU	LYS	THR	R1483	ALA	Y1245
A2526	Q2527	I2274	ARG	ASP	F1998	HIS	ASP	ALA	HIS	ARG	THR	R1483	ALA	D1246
Q2527	Q2528	I2274	ARG	ASP	V1999	MET	ASP	GLY	GLY	THR	GLY	R1483	ALA	F1247
S2529	E2416	G2282	LYS	GLU	S2009	VAL	GLU	LYS	ALA	ASP	THR	R1483	ALA	F1260
Q2530	L2430	LYS	GLY	LEU	I2010	VAL	LEU	THR	ALA	ASP	GLN	R1483	ALA	A1266
L2531	S2434	HIS	SER	LEU	L2014	PRO	TYR	LEU	ARG	PRO	GLY	R1483	ALA	R1269
V2532	K2449	THR	THR	GLN	F2020	ASP	ALA	ASP	ARG	LYS	GLY	R1483	ALA	Y1269
M2534	R2452	ALA	ARG	GLY	L2021	SER	GLU	GLY	THR	LYS	THR	R1483	ALA	A1266
D2535	R2452	ALA	ASN	ARG	V2027	THR	ALA	GLY	ALA	ASP	GLN	R1483	ALA	R1269
N2536	R2452	ASP	SER	GLY	P2028	ASP	ALA	GLY	ALA	ASP	GLY	R1483	ALA	G1273
S2537	P2461	ILE	SER	SER	Y2041	LYS	GLY	VAL	ARG	ASP	ALA	R1483	ALA	D1274
K2538	R2462	THR	GLN	SER	Q2053	THR	THR	THR	ARG	ASP	LYS	R1483	ALA	M1280
Y2539	Q2463	SER	LYS	SER	G2055	LEU	VAL	ASP	ASP	ASP	LYS	R1483	ALA	Y1297
N2540	Q2464	SER	GLY	ASP	PHE	PRO	GLU	GLY	ASP	ASP	LYS	R1483	ALA	I1302
E2541	K2465	SER	GLY	SER	PHE	LEU	GLY	GLY	ASP	ASP	GLY	R1483	ALA	Y1302
♦	W2465	SER	SER	LYS	G2055	SER	ILE	ILE	ASP	ASP	GLY	R1483	ALA	F1323
K2544	V2480	GLU	VAL	SER	G2055	LEU	SER	SER	ASP	ASP	GLY	R1483	ALA	♦
S2545	L2481	ASP	LEU	ILE	PHE	PRO	THR	THR	ASP	ASP	GLY	R1483	ALA	♦
F2546	L2481	GLN	SER	ASN	PHE	PRO	THR	THR	ASP	ASP	GLY	R1483	ALA	♦
♦	I2483	V2299	LEU	LEU	PHE	LEU	LEU	LEU	ASP	ASP	GLY	R1483	ALA	♦
G2547	I2483	P2300	LYS	ALA	PHE	LEU	LEU	LEU	ASP	ASP	GLY	R1483	ALA	♦
♦	W2486	LYS	LYS	ALA	G2055	TRP	GLU	GLU	ASP	ASP	GLY	R1483	ALA	♦
G2551	V2487	ALA	GLN	ALA	F2054	ASN	GLU	GLU	ASP	ASP	GLY	R1483	ALA	♦
A2552	W2487	SER	LYS	SER	G2055	LYS	LEU	LEU	ASP	ASP	GLY	R1483	ALA	♦
M2553	F2488	VAL	LYS	ASN	PHE	LEU	LEU	LEU	ASP	ASP	GLY	R1483	ALA	♦
Q2554	P2489	SER	GLN	ALA	PHE	LEU	LEU	LEU	ASP	ASP	GLY	R1483	ALA	♦
P2555	L2490	LYS	ARG	VAL	PHE	LEU	LEU	LEU	ASP	ASP	GLY	R1483	ALA	♦
L2556	♦	ARG	ARG	SER	SER	LEU	LEU	LEU	ASP	ASP	GLY	R1483	ALA	♦
E2557	♦	ARG	ARG	SER	SER	LEU	LEU	LEU	ASP	ASP	GLY	R1483	ALA	♦



• Molecule 1: Piezo-type mechanosensitive ion channel component 2

Chain C: 50% 15% 36%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	2721959	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	49.744	Depositor
Minimum map value	-19.493	Depositor
Average map value	0.078	Depositor
Map value standard deviation	1.367	Depositor
Recommended contour level	5.69	Depositor
Map size ($\text{\AA}$)	448.32, 448.32, 448.32	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.401, 1.401, 1.401	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.16	0/15321	0.35	0/20784
1	B	0.16	0/15321	0.35	0/20784
1	C	0.16	0/15321	0.35	0/20784
All	All	0.16	0/45963	0.35	0/62352

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	14908	0	15077	289	0
1	B	14908	0	15077	285	0
1	C	14908	0	15077	295	0
2	A	56	0	52	5	0
2	B	56	0	52	5	0
2	C	56	0	52	5	0
All	All	44892	0	45387	840	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 (840) 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:B:2650:PRO:HB2	1:B:2685:THR:HG22	1.33	1.11
1:C:2650:PRO:HB2	1:C:2685:THR:HG22	1.33	1.08
1:A:2650:PRO:HB2	1:A:2685:THR:HG22	1.33	1.06
1:A:2650:PRO:HB2	1:A:2685:THR:CG2	1.89	1.02
1:C:2650:PRO:HB2	1:C:2685:THR:CG2	1.89	1.02
1:B:2650:PRO:HB2	1:B:2685:THR:CG2	1.89	1.02
1:A:2753:LYS:NZ	1:B:2754:PHE:CE1	2.29	1.01
1:A:2754:PHE:CE1	1:C:2753:LYS:NZ	2.30	1.00
1:B:2753:LYS:NZ	1:C:2754:PHE:CE1	2.29	1.00
1:B:2622:LYS:HZ1	1:C:2607:GLN:HE22	1.09	0.99
1:A:2622:LYS:HZ1	1:B:2607:GLN:HE22	1.04	0.98
1:A:2622:LYS:NZ	1:B:2607:GLN:HE22	1.67	0.92
1:B:2622:LYS:NZ	1:C:2607:GLN:HE22	1.69	0.91
1:A:2607:GLN:HE22	1:C:2622:LYS:NZ	1.69	0.91
1:C:1040:ASN:OD1	1:C:1217:LYS:HA	1.80	0.81
1:A:2607:GLN:HE22	1:C:2622:LYS:HZ1	1.27	0.81
1:A:1040:ASN:OD1	1:A:1217:LYS:HA	1.80	0.81
1:B:1040:ASN:OD1	1:B:1217:LYS:HA	1.80	0.80
1:C:1992:SER:HG	1:C:2099:HIS:HD1	1.28	0.80
2:B:3002:NAG:H83	2:B:3002:NAG:H3	1.64	0.80
2:A:3002:NAG:H3	2:A:3002:NAG:H83	1.64	0.80
1:B:2753:LYS:NZ	1:C:2754:PHE:CD1	2.50	0.79
1:A:2753:LYS:NZ	1:B:2754:PHE:CD1	2.49	0.79
1:A:2754:PHE:CD1	1:C:2753:LYS:NZ	2.51	0.79
2:C:3002:NAG:H3	2:C:3002:NAG:H83	1.64	0.77
2:A:3002:NAG:H82	2:A:3002:NAG:C1	2.19	0.73
1:C:1030:ASN:OD1	1:C:1055:PRO:HB3	1.89	0.73
1:B:1030:ASN:OD1	1:B:1055:PRO:HB3	1.89	0.73
2:C:3002:NAG:C1	2:C:3002:NAG:H82	2.19	0.72
1:B:2670:LYS:HD3	1:B:2671:PRO:HD2	1.71	0.72
2:B:3002:NAG:C1	2:B:3002:NAG:H82	2.19	0.72
1:A:1030:ASN:OD1	1:A:1055:PRO:HB3	1.89	0.72
1:A:2670:LYS:HD3	1:A:2671:PRO:HD2	1.71	0.72
1:A:296:GLU:HG3	1:A:297:ALA:H	1.55	0.72
1:C:296:GLU:HG3	1:C:297:ALA:H	1.54	0.71
1:C:2021:LEU:HD11	1:C:2337:VAL:HG11	1.72	0.71
1:A:2021:LEU:HD11	1:A:2337:VAL:HG11	1.72	0.71
1:C:2670:LYS:HD3	1:C:2671:PRO:HD2	1.71	0.71
1:B:61:GLN:HE21	1:B:132:ALA:HB1	1.56	0.71
1:C:61:GLN:HE21	1:C:132:ALA:HB1	1.56	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2021:LEU:HD11	1:B:2337:VAL:HG11	1.72	0.70
1:B:296:GLU:HG3	1:B:297:ALA:H	1.54	0.70
1:B:1957:LYS:HD3	1:B:1960:HIS:HB3	1.74	0.70
1:A:1957:LYS:HD3	1:A:1960:HIS:HB3	1.74	0.70
1:A:2464:GLN:HG2	1:A:2465:LYS:H	1.57	0.70
1:C:1957:LYS:HD3	1:C:1960:HIS:HB3	1.74	0.69
1:A:61:GLN:HE21	1:A:132:ALA:HB1	1.56	0.69
1:B:2464:GLN:HG2	1:B:2465:LYS:H	1.57	0.69
1:C:2464:GLN:HG2	1:C:2465:LYS:H	1.57	0.68
1:A:576:GLU:OE2	1:A:578:LYS:NZ	2.28	0.67
1:C:2461:PRO:HD2	1:C:2464:GLN:HE22	1.60	0.67
1:C:2270:ASP:OD2	1:C:2310:GLN:NE2	2.28	0.67
1:A:2270:ASP:OD2	1:A:2310:GLN:NE2	2.28	0.66
1:A:2677:SER:O	1:A:2680:ASN:ND2	2.28	0.66
1:B:2270:ASP:OD2	1:B:2310:GLN:NE2	2.28	0.66
1:B:2461:PRO:HD2	1:B:2464:GLN:HE22	1.60	0.66
1:A:2461:PRO:HD2	1:A:2464:GLN:HE22	1.60	0.66
1:C:2677:SER:O	1:C:2680:ASN:ND2	2.28	0.66
2:A:3002:NAG:H3	2:A:3002:NAG:C8	2.26	0.66
1:B:2677:SER:O	1:B:2680:ASN:ND2	2.28	0.66
1:C:2560:GLU:HG3	1:C:2562:GLU:H	1.61	0.66
1:A:231:LEU:HD22	1:A:344:MET:HE2	1.78	0.66
1:B:576:GLU:OE2	1:B:578:LYS:NZ	2.28	0.65
2:B:3002:NAG:H3	2:B:3002:NAG:C8	2.26	0.65
1:B:231:LEU:HD22	1:B:344:MET:HE2	1.78	0.65
1:A:2622:LYS:NZ	1:B:2607:GLN:NE2	2.44	0.65
1:B:1155:ARG:NH2	1:B:1246:ASP:OD1	2.30	0.65
1:C:1155:ARG:NH2	1:C:1246:ASP:OD1	2.30	0.65
1:C:576:GLU:OE2	1:C:578:LYS:NZ	2.28	0.65
1:A:2560:GLU:HG3	1:A:2562:GLU:H	1.61	0.64
1:C:231:LEU:HD22	1:C:344:MET:HE2	1.78	0.64
1:B:2560:GLU:HG3	1:B:2562:GLU:H	1.61	0.64
2:C:3002:NAG:H3	2:C:3002:NAG:C8	2.26	0.64
1:B:2622:LYS:NZ	1:C:2607:GLN:NE2	2.45	0.64
1:C:38:LEU:HA	1:C:41:ILE:HD12	1.80	0.64
1:A:1708:GLU:O	1:A:1712:GLY:N	2.30	0.63
1:A:2607:GLN:NE2	1:C:2622:LYS:NZ	2.45	0.63
1:B:734:ARG:NH1	1:B:820:THR:O	2.32	0.63
1:B:2449:LYS:NZ	1:B:2775:ASP:OD2	2.32	0.63
1:A:38:LEU:HA	1:A:41:ILE:HD12	1.80	0.63
1:B:38:LEU:HA	1:B:41:ILE:HD12	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1952:ASP:HB3	1:B:1955:MET:HE1	1.81	0.63
1:B:2505:GLN:NE2	1:B:2562:GLU:O	2.32	0.62
1:C:734:ARG:NH1	1:C:820:THR:O	2.32	0.62
1:C:2449:LYS:NZ	1:C:2775:ASP:OD2	2.32	0.62
1:A:2449:LYS:NZ	1:A:2775:ASP:OD2	2.32	0.62
1:A:2505:GLN:NE2	1:A:2562:GLU:O	2.32	0.62
1:B:1708:GLU:O	1:B:1712:GLY:N	2.30	0.62
1:A:734:ARG:NH1	1:A:820:THR:O	2.32	0.62
1:C:1982:TYR:O	1:C:1986:ASN:ND2	2.33	0.62
1:C:1952:ASP:HB3	1:C:1955:MET:HE1	1.81	0.62
1:C:2505:GLN:NE2	1:C:2562:GLU:O	2.32	0.62
1:A:1155:ARG:NH2	1:A:1246:ASP:OD1	2.30	0.62
1:C:215:ILE:O	1:C:219:ILE:HG12	2.00	0.61
1:A:215:ILE:O	1:A:219:ILE:HG12	2.01	0.61
1:A:1952:ASP:HB3	1:A:1955:MET:HE1	1.81	0.61
1:B:215:ILE:O	1:B:219:ILE:HG12	2.01	0.61
1:C:1708:GLU:O	1:C:1712:GLY:N	2.30	0.61
1:B:1992:SER:OG	1:B:2099:HIS:ND1	2.33	0.60
1:C:2508:ASP:HB3	1:C:2607:GLN:HB3	1.83	0.60
1:A:224:LYS:O	1:A:228:THR:HG23	2.02	0.60
1:B:2535:ASP:O	1:B:2539:TYR:N	2.31	0.60
1:A:2508:ASP:HB3	1:A:2607:GLN:HB3	1.83	0.60
1:B:1982:TYR:O	1:B:1986:ASN:ND2	2.33	0.60
1:B:224:LYS:O	1:B:228:THR:HG23	2.02	0.60
1:B:1036:GLU:O	1:B:1040:ASN:ND2	2.28	0.59
1:A:2379:GLN:NE2	1:A:2383:GLY:O	2.35	0.59
1:B:980:TYR:O	1:B:984:ILE:HG12	2.03	0.59
1:A:503:CYS:HA	1:A:506:ILE:HG22	1.85	0.59
1:C:503:CYS:HA	1:C:506:ILE:HG22	1.85	0.59
1:A:1982:TYR:O	1:A:1986:ASN:ND2	2.33	0.59
1:C:224:LYS:O	1:C:228:THR:HG23	2.02	0.59
1:B:2274:ILE:HD11	1:B:2306:MET:HG2	1.85	0.58
1:C:2379:GLN:NE2	1:C:2383:GLY:O	2.35	0.58
1:A:505:LEU:HD13	1:A:530:LEU:HD23	1.84	0.58
1:B:505:LEU:HD13	1:B:530:LEU:HD23	1.84	0.58
1:C:75:ILE:O	1:C:78:HIS:NE2	2.36	0.58
1:C:284:ILE:O	1:C:288:LEU:HB3	2.04	0.58
1:A:980:TYR:O	1:A:984:ILE:HG12	2.03	0.58
1:B:75:ILE:O	1:B:78:HIS:NE2	2.36	0.58
1:B:934:THR:OG1	1:B:935:VAL:N	2.37	0.58
1:A:75:ILE:O	1:A:78:HIS:NE2	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:934:THR:OG1	1:A:935:VAL:N	2.37	0.58
1:A:1036:GLU:O	1:A:1040:ASN:ND2	2.28	0.58
1:C:505:LEU:HD13	1:C:530:LEU:HD23	1.84	0.58
1:B:503:CYS:HA	1:B:506:ILE:HG22	1.85	0.58
1:B:2508:ASP:HB3	1:B:2607:GLN:HB3	1.83	0.58
1:C:980:TYR:O	1:C:984:ILE:HG12	2.03	0.58
1:C:2536:ASN:OD1	1:C:2537:SER:N	2.37	0.58
1:B:284:ILE:O	1:B:288:LEU:HB3	2.04	0.58
1:C:2530:GLN:HB3	1:C:2568:GLU:HB3	1.86	0.58
1:C:2566:VAL:HG21	1:C:2711:PHE:HZ	1.69	0.58
1:B:2379:GLN:NE2	1:B:2383:GLY:O	2.35	0.58
1:A:284:ILE:O	1:A:288:LEU:HB3	2.04	0.57
1:A:967:ILE:HD11	1:A:1084:LEU:HD21	1.86	0.57
1:A:1992:SER:OG	1:A:2099:HIS:ND1	2.33	0.57
1:B:2566:VAL:HG21	1:B:2711:PHE:HZ	1.69	0.57
1:C:967:ILE:HD11	1:C:1084:LEU:HD21	1.86	0.57
1:B:2536:ASN:OD1	1:B:2537:SER:N	2.37	0.57
1:C:552:ASN:O	1:C:556:VAL:HG23	2.05	0.57
1:C:758:TYR:O	1:C:759:GLN:NE2	2.38	0.57
1:A:552:ASN:O	1:A:556:VAL:HG23	2.04	0.57
1:A:2566:VAL:HG21	1:A:2711:PHE:HZ	1.69	0.57
1:A:758:TYR:O	1:A:759:GLN:NE2	2.38	0.57
1:A:2530:GLN:HB3	1:A:2568:GLU:HB3	1.86	0.57
1:A:2535:ASP:O	1:A:2539:TYR:N	2.31	0.57
1:B:2530:GLN:HB3	1:B:2568:GLU:HB3	1.86	0.57
1:C:2274:ILE:HD11	1:C:2306:MET:HG2	1.85	0.57
1:B:967:ILE:HD11	1:B:1084:LEU:HD21	1.86	0.57
1:C:2508:ASP:OD1	1:C:2527:GLN:NE2	2.31	0.57
1:A:1677:VAL:O	1:A:1681:THR:HG23	2.06	0.56
1:A:2536:ASN:OD1	1:A:2537:SER:N	2.37	0.56
1:B:2517:GLY:O	1:C:2525:SER:OG	2.23	0.56
1:B:758:TYR:O	1:B:759:GLN:NE2	2.38	0.56
1:A:980:TYR:CZ	1:A:984:ILE:HD11	2.40	0.56
1:B:548:VAL:HG22	1:B:593:PHE:HB3	1.87	0.56
1:B:1677:VAL:O	1:B:1681:THR:HG23	2.05	0.56
1:C:548:VAL:HG22	1:C:593:PHE:HB3	1.88	0.56
1:C:1151:VAL:HG22	1:C:1245:TYR:HB3	1.87	0.56
1:B:552:ASN:O	1:B:556:VAL:HG23	2.04	0.56
1:A:548:VAL:HG22	1:A:593:PHE:HB3	1.87	0.56
1:A:2274:ILE:HD11	1:A:2306:MET:HG2	1.85	0.56
1:A:2304:LEU:HD11	1:C:2490:LEU:HB3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1151:VAL:HG22	1:B:1245:TYR:HB3	1.87	0.56
1:B:729:HIS:CD2	1:B:731:GLU:HB3	2.41	0.56
1:C:2710:ILE:HG22	1:C:2711:PHE:H	1.71	0.56
1:A:729:HIS:CD2	1:A:731:GLU:HB3	2.41	0.56
1:C:1677:VAL:O	1:C:1681:THR:HG23	2.05	0.56
1:B:343:VAL:O	1:B:347:THR:HG23	2.05	0.56
1:C:1155:ARG:NH2	1:C:1197:GLN:OE1	2.39	0.56
1:C:1483:ARG:NH1	1:C:2256:VAL:O	2.39	0.56
1:A:1155:ARG:NH2	1:A:1197:GLN:OE1	2.39	0.55
1:B:977:LEU:HG	1:B:978:PHE:H	1.71	0.55
1:A:1151:VAL:HG22	1:A:1245:TYR:HB3	1.87	0.55
1:B:980:TYR:CZ	1:B:984:ILE:HD11	2.40	0.55
1:A:1483:ARG:NH1	1:A:2256:VAL:O	2.39	0.55
1:B:2710:ILE:HG22	1:B:2711:PHE:H	1.71	0.55
1:C:729:HIS:CD2	1:C:731:GLU:HB3	2.41	0.55
1:C:1684:LEU:HD13	1:C:1687:ILE:HD11	1.87	0.55
1:A:346:TYR:O	1:A:350:THR:HG23	2.07	0.55
1:A:2490:LEU:HB3	1:B:2304:LEU:HD11	1.89	0.55
1:B:1155:ARG:NH2	1:B:1197:GLN:OE1	2.39	0.55
1:B:1684:LEU:HD13	1:B:1687:ILE:HD11	1.87	0.55
1:C:977:LEU:HG	1:C:978:PHE:H	1.71	0.55
1:C:343:VAL:O	1:C:347:THR:HG23	2.05	0.55
1:A:343:VAL:O	1:A:347:THR:HG23	2.05	0.55
1:C:346:TYR:O	1:C:350:THR:HG23	2.07	0.55
1:A:977:LEU:HG	1:A:978:PHE:H	1.71	0.55
1:A:1564:ARG:NH2	1:C:2452:ARG:NH2	2.54	0.55
1:A:2508:ASP:OD1	1:A:2527:GLN:NE2	2.31	0.55
1:B:1483:ARG:NH1	1:B:2256:VAL:O	2.39	0.55
1:C:980:TYR:CZ	1:C:984:ILE:HD11	2.40	0.55
1:C:2535:ASP:O	1:C:2539:TYR:N	2.31	0.55
1:A:251:LEU:HD11	1:A:552:ASN:HB2	1.89	0.55
1:A:1684:LEU:HD13	1:A:1687:ILE:HD11	1.87	0.55
1:A:2710:ILE:HG22	1:A:2711:PHE:H	1.71	0.55
1:B:346:TYR:O	1:B:350:THR:HG23	2.07	0.55
1:B:251:LEU:HD11	1:B:552:ASN:HB2	1.89	0.55
1:B:2508:ASP:OD1	1:B:2527:GLN:NE2	2.31	0.55
2:A:3002:NAG:C1	2:A:3002:NAG:C8	2.86	0.54
1:C:513:ILE:HG23	1:C:791:LEU:HD22	1.90	0.54
1:A:513:ILE:HG23	1:A:791:LEU:HD22	1.90	0.54
1:B:2452:ARG:NH2	1:C:1564:ARG:NH2	2.56	0.54
1:C:1036:GLU:O	1:C:1040:ASN:ND2	2.28	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:980:TYR:HD1	1:A:1198:TYR:HD2	1.56	0.54
1:C:2509:VAL:HG21	1:C:2567:ALA:HB1	1.90	0.54
1:A:2452:ARG:NH2	1:B:1564:ARG:NH2	2.55	0.54
1:A:2517:GLY:O	1:B:2525:SER:OG	2.22	0.54
1:B:15:LEU:HA	1:B:18:CYS:SG	2.48	0.54
1:B:243:SER:HA	1:B:246:TYR:HD2	1.73	0.54
1:B:2490:LEU:HB3	1:C:2304:LEU:HD11	1.88	0.54
1:B:2750:VAL:HG12	1:B:2754:PHE:CE2	2.43	0.54
1:C:243:SER:HA	1:C:246:TYR:HD2	1.73	0.54
1:A:716:MET:HB3	1:A:1015:MET:HE1	1.90	0.54
1:A:2509:VAL:HG21	1:A:2567:ALA:HB1	1.90	0.54
1:B:2340:ILE:HD12	1:B:2365:TRP:HH2	1.73	0.54
1:A:243:SER:HA	1:A:246:TYR:HD2	1.73	0.54
1:A:2525:SER:OG	1:C:2517:GLY:O	2.23	0.54
1:A:2750:VAL:HG12	1:A:2754:PHE:CE2	2.43	0.54
1:B:980:TYR:HD1	1:B:1198:TYR:HD2	1.56	0.54
1:B:2643:ASP:OD1	1:B:2646:SER:N	2.41	0.54
1:C:15:LEU:HA	1:C:18:CYS:SG	2.48	0.54
1:C:2464:GLN:HG2	1:C:2465:LYS:N	2.23	0.54
1:C:2750:VAL:HG12	1:C:2754:PHE:CE2	2.43	0.54
1:B:2602:PHE:O	1:B:2622:LYS:HB2	2.08	0.53
1:C:2602:PHE:O	1:C:2622:LYS:HB2	2.08	0.53
1:A:15:LEU:HA	1:A:18:CYS:SG	2.48	0.53
1:B:513:ILE:HG23	1:B:791:LEU:HD22	1.90	0.53
1:A:2672:ILE:HG21	1:A:2675:LEU:HD23	1.90	0.53
1:A:2513:ILE:HG13	1:A:2602:PHE:HD1	1.74	0.53
1:B:289:TYR:HA	1:B:292:GLN:HE21	1.73	0.53
1:B:2646:SER:OG	1:B:2647:SER:N	2.42	0.53
1:C:251:LEU:HD11	1:C:552:ASN:HB2	1.89	0.53
1:C:716:MET:HB3	1:C:1015:MET:HE1	1.90	0.53
1:A:2602:PHE:O	1:A:2622:LYS:HB2	2.08	0.53
1:B:2509:VAL:HG21	1:B:2567:ALA:HB1	1.90	0.53
1:C:289:TYR:HA	1:C:292:GLN:HE21	1.73	0.53
1:C:934:THR:OG1	1:C:935:VAL:N	2.37	0.53
1:C:2518:TYR:OH	1:C:2590:GLU:OE1	2.25	0.53
1:B:716:MET:HB3	1:B:1015:MET:HE1	1.90	0.53
1:A:2553:MET:O	1:A:2557:GLU:HG2	2.09	0.53
1:B:283:LEU:HD21	1:B:341:LEU:HB3	1.91	0.53
1:A:289:TYR:HA	1:A:292:GLN:HE21	1.73	0.53
1:A:1689:ARG:NH1	1:A:1693:ASP:OD2	2.42	0.53
1:B:1689:ARG:NH1	1:B:1693:ASP:OD2	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:980:TYR:HD1	1:C:1198:TYR:HD2	1.56	0.53
1:C:2340:ILE:HD12	1:C:2365:TRP:HH2	1.73	0.53
1:A:283:LEU:HD21	1:A:341:LEU:HB3	1.91	0.53
1:A:2607:GLN:HE22	1:C:2622:LYS:HZ3	1.53	0.53
1:B:2686:ILE:HG22	1:B:2703:LEU:HD22	1.91	0.53
1:C:2686:ILE:HG22	1:C:2703:LEU:HD22	1.91	0.53
1:B:2553:MET:O	1:B:2557:GLU:HG2	2.09	0.53
1:C:2513:ILE:HG13	1:C:2602:PHE:HD1	1.74	0.53
1:C:2643:ASP:OD1	1:C:2646:SER:N	2.41	0.53
1:C:2646:SER:OG	1:C:2647:SER:N	2.42	0.53
2:C:3002:NAG:C1	2:C:3002:NAG:C8	2.86	0.53
1:A:2340:ILE:HD12	1:A:2365:TRP:HH2	1.73	0.52
1:C:2672:ILE:HG21	1:C:2675:LEU:HD23	1.90	0.52
1:A:2646:SER:OG	1:A:2647:SER:N	2.42	0.52
1:A:2686:ILE:HG22	1:A:2703:LEU:HD22	1.91	0.52
1:C:1689:ARG:NH1	1:C:1693:ASP:OD2	2.42	0.52
1:B:1269:ARG:HA	1:B:1273:GLY:HA3	1.92	0.52
1:C:283:LEU:HD21	1:C:341:LEU:HB3	1.91	0.52
1:C:2501:GLY:HA2	1:C:2728:SER:HA	1.92	0.52
1:A:223:GLY:O	1:A:227:VAL:HG23	2.10	0.52
1:A:2464:GLN:HG2	1:A:2465:LYS:N	2.23	0.52
1:C:2553:MET:O	1:C:2557:GLU:HG2	2.09	0.52
1:A:2643:ASP:OD1	1:A:2646:SER:N	2.41	0.52
1:B:52:MET:HA	1:B:55:HIS:HD1	1.75	0.52
1:B:1716:THR:O	1:B:1719:SER:N	2.40	0.52
1:C:2330:VAL:HG12	1:C:2380:ILE:HD13	1.92	0.52
1:A:2501:GLY:HA2	1:A:2728:SER:HA	1.92	0.52
1:A:2330:VAL:HG12	1:A:2380:ILE:HD13	1.92	0.52
1:B:1199:PHE:O	1:B:1202:ILE:HG22	2.10	0.52
1:C:1199:PHE:O	1:C:1202:ILE:HG22	2.10	0.52
1:B:770:MET:HE2	1:B:770:MET:HA	1.92	0.52
1:B:2330:VAL:HG12	1:B:2380:ILE:HD13	1.92	0.52
1:B:2672:ILE:HG21	1:B:2675:LEU:HD23	1.91	0.52
1:C:1280:MET:HA	1:C:1356:ILE:HD11	1.92	0.52
1:A:12:ARG:O	1:A:16:PRO:HD2	2.10	0.52
1:A:2480:VAL:HA	1:A:2483:ILE:HG22	1.92	0.52
1:C:2608:ARG:NH1	1:C:2664:PRO:O	2.33	0.52
1:A:2515:LEU:HD12	1:A:2600:VAL:HG13	1.93	0.51
1:B:12:ARG:O	1:B:16:PRO:HD2	2.10	0.51
1:B:1574:ASP:N	1:B:1574:ASP:OD1	2.43	0.51
1:B:2501:GLY:HA2	1:B:2728:SER:HA	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2515:LEU:HD12	1:C:2600:VAL:HG13	1.93	0.51
1:A:1141:LEU:HD11	1:A:1260:PHE:HZ	1.76	0.51
1:A:1269:ARG:HA	1:A:1273:GLY:HA3	1.92	0.51
1:A:1280:MET:HA	1:A:1356:ILE:HD11	1.92	0.51
1:B:52:MET:O	1:B:55:HIS:ND1	2.43	0.51
1:C:770:MET:HE2	1:C:770:MET:HA	1.92	0.51
1:A:1574:ASP:OD1	1:A:1574:ASP:N	2.43	0.51
1:A:1716:THR:O	1:A:1719:SER:N	2.40	0.51
1:B:2513:ILE:HG13	1:B:2602:PHE:HD1	1.74	0.51
1:C:1141:LEU:HD11	1:C:1260:PHE:HZ	1.75	0.51
1:C:2685:THR:HB	1:C:2704:ASN:HB3	1.93	0.51
1:A:52:MET:O	1:A:55:HIS:ND1	2.43	0.51
1:A:1199:PHE:O	1:A:1202:ILE:HG22	2.10	0.51
1:A:1330:ILE:HD12	1:A:1330:ILE:H	1.75	0.51
1:B:2480:VAL:HA	1:B:2483:ILE:HG22	1.92	0.51
1:A:217:ASN:HA	1:A:220:THR:HG22	1.93	0.51
1:B:1280:MET:HA	1:B:1356:ILE:HD11	1.92	0.51
1:B:1330:ILE:H	1:B:1330:ILE:HD12	1.76	0.51
1:B:1141:LEU:HD11	1:B:1260:PHE:HZ	1.75	0.51
1:C:2027:VAL:HB	1:C:2028:PRO:HD3	1.93	0.51
1:B:223:GLY:O	1:B:227:VAL:HG23	2.10	0.51
1:B:2685:THR:HB	1:B:2704:ASN:HB3	1.93	0.51
1:C:1141:LEU:HD13	1:C:1179:ILE:HD11	1.93	0.51
1:C:1269:ARG:HA	1:C:1273:GLY:HA3	1.92	0.51
1:C:52:MET:O	1:C:55:HIS:ND1	2.43	0.51
1:C:223:GLY:O	1:C:227:VAL:HG23	2.10	0.51
1:A:1141:LEU:HD13	1:A:1179:ILE:HD11	1.93	0.50
1:A:770:MET:HE2	1:A:770:MET:HA	1.92	0.50
1:A:2685:THR:HB	1:A:2704:ASN:HB3	1.93	0.50
1:B:2464:GLN:HG2	1:B:2465:LYS:N	2.23	0.50
1:C:2524:MET:HG2	1:C:2569:LEU:HB3	1.94	0.50
1:B:12:ARG:NE	1:B:46:GLU:OE2	2.44	0.50
1:B:217:ASN:HA	1:B:220:THR:HG22	1.93	0.50
1:C:12:ARG:O	1:C:16:PRO:HD2	2.10	0.50
1:C:1330:ILE:HD12	1:C:1330:ILE:H	1.76	0.50
1:C:2480:VAL:HA	1:C:2483:ILE:HG22	1.93	0.50
1:C:2551:GLY:O	1:C:2554:GLN:NE2	2.31	0.50
1:A:2524:MET:HG2	1:A:2569:LEU:HB3	1.94	0.50
1:B:2524:MET:HG2	1:B:2569:LEU:HB3	1.94	0.50
1:C:217:ASN:HA	1:C:220:THR:HG22	1.93	0.50
1:A:2608:ARG:NH1	1:A:2664:PRO:O	2.33	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:LEU:HD13	1:A:567:GLU:HG2	1.93	0.50
1:B:2027:VAL:HB	1:B:2028:PRO:HD3	1.93	0.50
1:B:2515:LEU:HD12	1:B:2600:VAL:HG13	1.93	0.50
1:A:12:ARG:NE	1:A:46:GLU:OE2	2.44	0.50
1:A:2585:GLN:HA	1:A:2588:ILE:HG12	1.94	0.50
1:B:257:TRP:O	1:B:598:ARG:NH1	2.45	0.50
1:C:257:TRP:O	1:C:598:ARG:NH1	2.45	0.50
1:C:1211:ASP:OD1	1:C:1212:TYR:N	2.38	0.50
1:A:1707:ARG:NE	1:A:1961:ASP:OD2	2.45	0.49
1:B:565:LEU:HD13	1:B:567:GLU:HG2	1.93	0.49
1:B:2504:ASN:O	1:B:2724:ASN:ND2	2.45	0.49
1:B:2271:PHE:HA	1:B:2274:ILE:HG22	1.94	0.49
1:A:2607:GLN:NE2	1:C:2622:LYS:HZ3	2.09	0.49
1:C:12:ARG:NE	1:C:46:GLU:OE2	2.44	0.49
1:C:2566:VAL:HG21	1:C:2711:PHE:CZ	2.47	0.49
1:A:257:TRP:O	1:A:598:ARG:NH1	2.45	0.49
1:A:1173:ARG:HB2	1:A:1179:ILE:HG22	1.94	0.49
1:B:2020:PHE:HZ	1:B:2370:CYS:HB3	1.78	0.49
1:A:2027:VAL:HB	1:A:2028:PRO:HD3	1.93	0.49
1:A:2504:ASN:O	1:A:2724:ASN:ND2	2.45	0.49
1:C:1707:ARG:NE	1:C:1961:ASP:OD2	2.45	0.49
1:C:2504:ASN:O	1:C:2724:ASN:ND2	2.45	0.49
1:C:2585:GLN:HA	1:C:2588:ILE:HG12	1.94	0.49
1:A:18:CYS:HA	1:A:21:VAL:HG22	1.94	0.49
1:B:1028:SER:OG	1:B:1055:PRO:HB2	2.13	0.49
1:B:1563:VAL:HG13	1:B:1564:ARG:HG3	1.95	0.49
1:C:565:LEU:HD13	1:C:567:GLU:HG2	1.93	0.49
1:C:1563:VAL:HG13	1:C:1564:ARG:HG3	1.95	0.49
1:A:942:GLU:HG3	1:A:946:LYS:HE3	1.95	0.49
1:A:2020:PHE:HZ	1:A:2370:CYS:HB3	1.78	0.49
1:B:942:GLU:HG3	1:B:946:LYS:HE3	1.95	0.49
1:B:1141:LEU:HD13	1:B:1179:ILE:HD11	1.93	0.49
1:B:1707:ARG:NE	1:B:1961:ASP:OD2	2.46	0.49
1:C:942:GLU:HG3	1:C:946:LYS:HE3	1.95	0.49
1:C:1028:SER:OG	1:C:1055:PRO:HB2	2.13	0.49
1:A:1028:SER:OG	1:A:1055:PRO:HB2	2.13	0.49
1:A:2566:VAL:HG21	1:A:2711:PHE:CZ	2.47	0.49
1:B:2585:GLN:HA	1:B:2588:ILE:HG12	1.94	0.49
1:B:18:CYS:HA	1:B:21:VAL:HG22	1.94	0.48
1:B:2566:VAL:HG21	1:B:2711:PHE:CZ	2.47	0.48
1:A:2271:PHE:HA	1:A:2274:ILE:HG22	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:CYS:HA	1:C:21:VAL:HG22	1.94	0.48
1:C:1333:PHE:O	1:C:1369:TYR:OH	2.30	0.48
1:A:1429:ILE:HG13	1:A:1429:ILE:O	2.14	0.48
1:C:2020:PHE:HZ	1:C:2370:CYS:HB3	1.78	0.48
1:C:2753:LYS:HD2	1:C:2753:LYS:O	2.14	0.48
1:C:1173:ARG:HB2	1:C:1179:ILE:HG22	1.95	0.48
1:C:2610:MET:HE3	1:C:2611:THR:H	1.79	0.48
1:B:1173:ARG:HB2	1:B:1179:ILE:HG22	1.94	0.48
1:C:1716:THR:O	1:C:1719:SER:N	2.40	0.48
1:C:2507:LEU:HD21	1:C:2610:MET:HG2	1.96	0.48
1:A:1037:ASN:O	1:A:1217:LYS:HB2	2.14	0.48
1:A:1563:VAL:HG13	1:A:1564:ARG:HG3	1.95	0.48
1:A:2563:ASP:O	1:A:2724:ASN:N	2.46	0.48
1:B:2518:TYR:OH	1:B:2590:GLU:OE1	2.25	0.48
1:A:1955:MET:SD	1:A:1955:MET:N	2.87	0.48
1:B:2563:ASP:O	1:B:2724:ASN:N	2.46	0.48
1:B:2610:MET:HE3	1:B:2611:THR:H	1.79	0.48
1:C:1955:MET:SD	1:C:1955:MET:N	2.87	0.48
1:C:2271:PHE:HA	1:C:2274:ILE:HG22	1.94	0.48
1:C:2603:SER:CB	1:C:2622:LYS:HB3	2.44	0.48
1:A:2753:LYS:HD2	1:A:2753:LYS:O	2.14	0.48
1:B:1955:MET:SD	1:B:1955:MET:N	2.87	0.48
1:C:1429:ILE:O	1:C:1429:ILE:HG13	2.14	0.48
1:A:1991:ARG:O	1:A:1995:VAL:HG23	2.14	0.48
1:C:2534:MET:HE2	1:C:2538:LYS:HB3	1.96	0.48
1:A:2534:MET:HE2	1:A:2538:LYS:HB3	1.96	0.47
1:C:1991:ARG:O	1:C:1995:VAL:HG23	2.14	0.47
1:C:2563:ASP:O	1:C:2724:ASN:N	2.46	0.47
1:A:1968:GLU:O	1:A:1972:VAL:HG13	2.15	0.47
1:B:2603:SER:CB	1:B:2622:LYS:HB3	2.44	0.47
1:C:39:LEU:HG	1:C:345:TYR:CZ	2.50	0.47
1:B:1367:ILE:HD11	1:B:1439:LEU:HB3	1.97	0.47
1:C:1574:ASP:OD1	1:C:1574:ASP:N	2.43	0.47
1:A:2610:MET:HE3	1:A:2611:THR:H	1.79	0.47
1:C:555:LEU:HD21	1:C:587:ILE:HD13	1.97	0.47
1:C:1037:ASN:O	1:C:1217:LYS:HB2	2.14	0.47
1:B:2507:LEU:HD21	1:B:2610:MET:HG2	1.96	0.47
1:B:2534:MET:HE2	1:B:2538:LYS:HB3	1.96	0.47
1:A:231:LEU:HB3	1:A:250:PHE:HB2	1.97	0.47
1:A:541:MET:HB3	1:A:600:HIS:CD2	2.50	0.47
1:B:231:LEU:HB3	1:B:250:PHE:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1968:GLU:O	1:B:1972:VAL:HG13	2.15	0.47
1:A:14:LEU:HD12	1:A:14:LEU:H	1.80	0.47
1:A:39:LEU:HG	1:A:345:TYR:CZ	2.50	0.47
1:A:1018:GLN:HG3	1:A:1070:LEU:HD13	1.96	0.47
1:A:1333:PHE:O	1:A:1369:TYR:OH	2.30	0.47
1:A:1969:LYS:HA	1:A:1972:VAL:HG22	1.96	0.47
1:A:2009:SER:OG	1:A:2010:ILE:N	2.47	0.47
1:A:2507:LEU:HD21	1:A:2610:MET:HG2	1.96	0.47
1:A:2518:TYR:OH	1:A:2590:GLU:OE1	2.25	0.47
1:A:2603:SER:CB	1:A:2622:LYS:HB3	2.44	0.47
1:B:1333:PHE:O	1:B:1369:TYR:OH	2.30	0.47
1:B:1991:ARG:O	1:B:1995:VAL:HG23	2.14	0.47
1:B:2753:LYS:O	1:B:2753:LYS:HD2	2.14	0.47
1:C:541:MET:HB3	1:C:600:HIS:CD2	2.50	0.47
1:C:1968:GLU:O	1:C:1972:VAL:HG13	2.15	0.47
1:C:2462:ARG:HG3	1:C:2463:GLY:H	1.79	0.47
1:B:39:LEU:HG	1:B:345:TYR:CZ	2.50	0.47
1:B:1969:LYS:HA	1:B:1972:VAL:HG22	1.97	0.47
1:B:2009:SER:OG	1:B:2010:ILE:N	2.47	0.47
1:A:50:ALA:HB3	1:A:53:GLN:HE21	1.80	0.47
1:B:541:MET:HB3	1:B:600:HIS:CD2	2.50	0.47
1:B:1429:ILE:HG13	1:B:1429:ILE:O	2.14	0.47
1:C:1969:LYS:HA	1:C:1972:VAL:HG22	1.96	0.47
1:A:1323:PHE:HB2	1:A:1341:CYS:SG	2.55	0.47
1:A:1956:SER:O	1:A:1956:SER:OG	2.33	0.47
1:B:339:ILE:HG13	1:B:340:LEU:N	2.31	0.47
1:B:1018:GLN:HG3	1:B:1070:LEU:HD13	1.96	0.47
1:B:2608:ARG:HG2	1:B:2608:ARG:HH21	1.79	0.47
1:C:1269:ARG:HG3	1:C:1274:ASP:H	1.80	0.47
1:A:2608:ARG:HH21	1:A:2608:ARG:HG2	1.79	0.46
1:B:1037:ASN:O	1:B:1217:LYS:HB2	2.14	0.46
1:B:2551:GLY:O	1:B:2554:GLN:NE2	2.31	0.46
1:C:14:LEU:H	1:C:14:LEU:HD12	1.80	0.46
1:C:231:LEU:HB3	1:C:250:PHE:HB2	1.97	0.46
1:C:797:ILE:HB	1:C:798:PRO:HD3	1.98	0.46
1:C:2009:SER:OG	1:C:2010:ILE:N	2.47	0.46
1:A:284:ILE:O	1:A:288:LEU:CB	2.64	0.46
1:B:14:LEU:HD12	1:B:14:LEU:H	1.80	0.46
1:A:2673:LYS:HZ2	1:A:2678:GLU:H	1.63	0.46
1:B:741:TRP:HB2	1:B:809:LEU:HD12	1.98	0.46
1:B:797:ILE:HB	1:B:798:PRO:HD3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1323:PHE:HB2	1:B:1341:CYS:SG	2.55	0.46
2:B:3002:NAG:C1	2:B:3002:NAG:C8	2.86	0.46
1:C:2608:ARG:HG2	1:C:2608:ARG:HH21	1.79	0.46
1:B:555:LEU:HD21	1:B:587:ILE:HD13	1.97	0.46
1:A:555:LEU:HD21	1:A:587:ILE:HD13	1.97	0.46
1:B:2535:ASP:HB3	1:B:2538:LYS:HB2	1.97	0.46
1:B:2608:ARG:NH1	1:B:2664:PRO:O	2.33	0.46
1:C:339:ILE:HG13	1:C:340:LEU:N	2.31	0.46
1:B:1269:ARG:HG3	1:B:1274:ASP:H	1.81	0.46
1:B:1051:LEU:HD23	1:B:1056:VAL:HG11	1.98	0.46
1:B:2462:ARG:HG3	1:B:2463:GLY:H	1.80	0.46
1:C:211:LEU:HA	1:C:214:PHE:CD1	2.51	0.46
1:C:1323:PHE:HB2	1:C:1341:CYS:SG	2.55	0.46
1:B:2519:GLN:HE22	1:B:2578:THR:HG22	1.81	0.46
1:C:1051:LEU:HD23	1:C:1056:VAL:HG11	1.98	0.46
1:C:2535:ASP:HB3	1:C:2538:LYS:HB2	1.97	0.46
1:A:211:LEU:HA	1:A:214:PHE:CD1	2.51	0.46
1:A:339:ILE:HG13	1:A:340:LEU:N	2.31	0.46
1:A:1367:ILE:HD11	1:A:1439:LEU:HB3	1.97	0.46
1:B:1366:LEU:HG	1:B:1439:LEU:HD21	1.98	0.46
1:C:264:ASP:CG	1:C:265:PRO:HD2	2.41	0.46
1:C:1018:GLN:HG3	1:C:1070:LEU:HD13	1.96	0.46
1:C:1323:PHE:CD1	1:C:2090:LEU:HD13	2.51	0.46
1:C:1367:ILE:HD11	1:C:1439:LEU:HB3	1.97	0.46
1:A:797:ILE:HB	1:A:798:PRO:HD3	1.98	0.46
1:A:2462:ARG:HG3	1:A:2463:GLY:H	1.80	0.46
1:A:2519:GLN:HE22	1:A:2578:THR:HG22	1.81	0.46
1:B:284:ILE:O	1:B:288:LEU:CB	2.64	0.46
1:C:2566:VAL:HB	1:C:2719:GLU:OE2	2.16	0.46
1:A:952:TRP:HB3	1:A:1094:GLN:NE2	2.31	0.45
1:A:1473:GLN:O	1:A:1477:VAL:HG13	2.16	0.45
1:B:211:LEU:HA	1:B:214:PHE:CD1	2.51	0.45
1:B:1323:PHE:CD1	1:B:2090:LEU:HD13	2.51	0.45
1:C:284:ILE:O	1:C:288:LEU:CB	2.63	0.45
1:C:952:TRP:HB3	1:C:1094:GLN:NE2	2.32	0.45
1:A:1269:ARG:HG3	1:A:1274:ASP:H	1.80	0.45
1:A:2808:ARG:NH1	1:C:2771:LEU:HD23	2.31	0.45
1:C:741:TRP:HB2	1:C:809:LEU:HD12	1.97	0.45
1:A:251:LEU:HD21	1:A:552:ASN:HD22	1.81	0.45
1:A:264:ASP:CG	1:A:265:PRO:HD2	2.41	0.45
1:A:1706:THR:HA	1:A:1709:ILE:HG22	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2574:ASN:HA	1:C:2583:SER:HB3	1.98	0.45
1:B:251:LEU:HD21	1:B:552:ASN:HD22	1.81	0.45
1:B:1706:THR:HA	1:B:1709:ILE:HG22	1.99	0.45
1:A:561:TRP:CE3	1:A:568:ILE:HD12	2.52	0.45
1:A:1366:LEU:HG	1:A:1439:LEU:HD21	1.98	0.45
1:B:952:TRP:HB3	1:B:1094:GLN:NE2	2.32	0.45
1:C:1366:LEU:HG	1:C:1439:LEU:HD21	1.98	0.45
1:A:2535:ASP:HB3	1:A:2538:LYS:HB2	1.97	0.45
1:C:2519:GLN:HE22	1:C:2578:THR:HG22	1.81	0.45
1:A:1323:PHE:CD1	1:A:2090:LEU:HD13	2.51	0.45
1:A:2771:LEU:HD23	1:B:2808:ARG:NH1	2.32	0.45
1:B:2583:SER:HB3	1:C:2574:ASN:HA	1.97	0.45
1:B:2673:LYS:HZ2	1:B:2678:GLU:H	1.65	0.45
1:A:2566:VAL:HB	1:A:2719:GLU:OE2	2.16	0.45
1:C:1230:TYR:OH	1:C:1239:ASN:O	2.35	0.45
1:A:31:SER:HA	1:A:34:TYR:CD2	2.52	0.45
1:A:2583:SER:HB3	1:B:2574:ASN:HA	1.98	0.45
1:B:264:ASP:CG	1:B:265:PRO:HD2	2.41	0.45
1:B:2364:LEU:O	1:B:2368:VAL:HG22	2.17	0.45
1:B:2391:ASN:HB3	1:B:2394:THR:CG2	2.47	0.45
1:A:2391:ASN:HB3	1:A:2394:THR:CG2	2.47	0.45
1:B:50:ALA:HB3	1:B:53:GLN:HE21	1.80	0.45
1:B:1037:ASN:OD1	2:B:3003:NAG:O7	2.35	0.45
1:B:2566:VAL:HB	1:B:2719:GLU:OE2	2.16	0.45
1:C:555:LEU:HD12	1:C:555:LEU:HA	1.83	0.45
1:C:561:TRP:CE3	1:C:568:ILE:HD12	2.52	0.45
1:C:1215:ARG:HH12	1:C:1235:ILE:HG21	1.82	0.45
1:C:1473:GLN:O	1:C:1477:VAL:HG13	2.16	0.45
1:A:741:TRP:HB2	1:A:809:LEU:HD12	1.97	0.44
1:A:1302:TYR:HA	1:A:1970:PHE:CZ	2.52	0.44
1:A:2014:LEU:HD22	1:A:2041:TYR:CZ	2.52	0.44
1:A:2482:LEU:O	1:A:2486:VAL:HG12	2.17	0.44
1:C:31:SER:HA	1:C:34:TYR:CD2	2.52	0.44
1:A:960:ILE:HD13	1:A:996:ARG:HD3	1.99	0.44
1:A:1297:ILE:HD13	1:A:1457:ASP:HB2	2.00	0.44
1:A:2540:ASN:O	1:A:2544:LYS:HG2	2.17	0.44
1:B:2482:LEU:O	1:B:2486:VAL:HG12	2.17	0.44
1:B:2540:ASN:O	1:B:2544:LYS:HG2	2.17	0.44
1:C:960:ILE:HD13	1:C:996:ARG:HD3	1.99	0.44
1:C:1037:ASN:OD1	2:C:3003:NAG:O7	2.35	0.44
1:B:960:ILE:HD13	1:B:996:ARG:HD3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2014:LEU:HD22	1:B:2041:TYR:CZ	2.52	0.44
1:B:2650:PRO:HB2	1:B:2685:THR:HG21	1.91	0.44
1:A:705:GLU:O	1:A:712:LYS:NZ	2.43	0.44
1:A:1037:ASN:OD1	2:A:3003:NAG:O7	2.35	0.44
1:A:2344:MET:HE3	1:A:2344:MET:HB3	1.91	0.44
1:A:2764:HIS:HA	1:B:2768:PHE:CE2	2.53	0.44
1:B:31:SER:HA	1:B:34:TYR:CD2	2.52	0.44
1:B:705:GLU:O	1:B:712:LYS:NZ	2.43	0.44
1:B:1302:TYR:HA	1:B:1970:PHE:CZ	2.52	0.44
1:B:1473:GLN:O	1:B:1477:VAL:HG13	2.16	0.44
1:C:50:ALA:HB3	1:C:53:GLN:HE21	1.80	0.44
1:A:2364:LEU:O	1:A:2368:VAL:HG22	2.17	0.44
1:A:2603:SER:OG	1:A:2622:LYS:HB3	2.18	0.44
1:B:561:TRP:HE3	1:B:568:ILE:HD12	1.83	0.44
1:B:2462:ARG:HD2	1:B:2462:ARG:HA	1.75	0.44
1:B:2603:SER:OG	1:B:2622:LYS:HB3	2.18	0.44
1:B:2771:LEU:HD23	1:C:2808:ARG:NH1	2.32	0.44
1:C:251:LEU:HD21	1:C:552:ASN:HD22	1.81	0.44
1:C:2053:GLN:HE22	1:C:2082:LYS:HA	1.83	0.44
1:C:2364:LEU:O	1:C:2368:VAL:HG22	2.17	0.44
1:C:2391:ASN:HB3	1:C:2394:THR:CG2	2.47	0.44
1:A:561:TRP:HE3	1:A:568:ILE:HD12	1.82	0.44
1:A:1230:TYR:OH	1:A:1239:ASN:O	2.35	0.44
1:C:1706:THR:HA	1:C:1709:ILE:HG22	1.99	0.44
1:C:2753:LYS:HD2	1:C:2753:LYS:C	2.42	0.44
1:A:1051:LEU:HD23	1:A:1056:VAL:HG11	1.98	0.44
1:B:1155:ARG:HH22	1:B:1197:GLN:CD	2.26	0.44
1:B:2753:LYS:HD2	1:B:2753:LYS:C	2.42	0.44
1:C:1302:TYR:HA	1:C:1970:PHE:CZ	2.52	0.44
1:C:2014:LEU:HD22	1:C:2041:TYR:CZ	2.52	0.44
1:C:2265:LEU:HD23	1:C:2265:LEU:HA	1.82	0.44
1:A:2753:LYS:HD2	1:A:2753:LYS:C	2.42	0.44
1:B:561:TRP:CE3	1:B:568:ILE:HD12	2.52	0.44
1:A:1215:ARG:HH12	1:A:1235:ILE:HG21	1.82	0.44
1:B:1673:PHE:O	1:B:1677:VAL:HG13	2.18	0.44
1:C:571:VAL:HG11	1:C:574:PHE:HB2	2.00	0.44
1:A:1155:ARG:HH22	1:A:1197:GLN:CD	2.26	0.43
1:A:2299:VAL:HB	1:A:2300:PRO:HD3	2.00	0.43
1:B:2753:LYS:NZ	1:C:2754:PHE:CZ	2.61	0.43
1:C:968:ILE:HG13	1:C:1247:PHE:CD1	2.53	0.43
1:A:679:LEU:O	1:A:683:VAL:HG22	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1154:GLN:NE2	1:A:1245:TYR:OH	2.51	0.43
1:A:1996:CYS:HA	1:A:1999:VAL:HG12	2.00	0.43
1:B:1215:ARG:HH12	1:B:1235:ILE:HG21	1.82	0.43
1:B:1962:ASP:OD1	1:B:1962:ASP:N	2.49	0.43
1:B:2053:GLN:HE22	1:B:2082:LYS:HA	1.83	0.43
1:C:32:PHE:HE1	1:C:284:ILE:HD12	1.84	0.43
1:C:2461:PRO:HD2	1:C:2464:GLN:NE2	2.31	0.43
1:C:2482:LEU:O	1:C:2486:VAL:HG12	2.17	0.43
1:A:2395:LYS:HE2	1:A:2395:LYS:HB3	1.89	0.43
1:B:968:ILE:HG13	1:B:1247:PHE:CD1	2.53	0.43
1:B:2299:VAL:HB	1:B:2300:PRO:HD3	2.00	0.43
1:C:2603:SER:OG	1:C:2622:LYS:HB3	2.18	0.43
1:A:968:ILE:HG13	1:A:1247:PHE:CD1	2.53	0.43
1:B:1435:CYS:O	1:B:1439:LEU:HD13	2.19	0.43
1:B:2020:PHE:CZ	1:B:2370:CYS:HB3	2.54	0.43
1:C:217:ASN:O	1:C:221:THR:HG23	2.19	0.43
1:C:1177:LYS:HE3	1:C:1177:LYS:HB2	1.87	0.43
1:C:1673:PHE:O	1:C:1677:VAL:HG13	2.18	0.43
1:C:1957:LYS:HB3	1:C:1957:LYS:HE3	1.83	0.43
1:A:1435:CYS:O	1:A:1439:LEU:HD13	2.19	0.43
1:B:1721:HIS:HA	1:B:1724:TYR:CD1	2.53	0.43
1:C:1154:GLN:NE2	1:C:1245:TYR:OH	2.51	0.43
1:C:1996:CYS:HA	1:C:1999:VAL:HG12	2.00	0.43
1:C:2540:ASN:O	1:C:2544:LYS:HG2	2.17	0.43
1:A:32:PHE:HE1	1:A:284:ILE:HD12	1.84	0.43
1:A:2462:ARG:HD2	1:A:2462:ARG:HA	1.75	0.43
1:B:32:PHE:HE1	1:B:284:ILE:HD12	1.84	0.43
1:A:2053:GLN:HE22	1:A:2082:LYS:HA	1.83	0.43
1:B:571:VAL:HG11	1:B:574:PHE:HB2	2.00	0.43
1:B:1721:HIS:HA	1:B:1724:TYR:CE1	2.54	0.43
1:B:1996:CYS:HA	1:B:1999:VAL:HG12	2.00	0.43
1:C:679:LEU:O	1:C:683:VAL:HG22	2.19	0.43
1:C:1962:ASP:OD1	1:C:1962:ASP:N	2.49	0.43
1:A:217:ASN:O	1:A:221:THR:HG23	2.19	0.43
1:A:2020:PHE:CZ	1:A:2370:CYS:HB3	2.54	0.43
1:A:1721:HIS:HA	1:A:1724:TYR:CD1	2.53	0.43
1:B:2271:PHE:O	1:B:2274:ILE:HG22	2.19	0.43
1:C:2299:VAL:HB	1:C:2300:PRO:HD3	2.00	0.43
1:C:2673:LYS:HZ2	1:C:2678:GLU:H	1.66	0.43
1:A:1363:TRP:O	1:A:1367:ILE:HG12	2.19	0.43
1:A:2587:MET:O	1:A:2590:GLU:HG2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2768:PHE:CE2	1:C:2764:HIS:HA	2.53	0.43
1:B:1297:ILE:HD13	1:B:1457:ASP:HB2	2.00	0.43
1:C:561:TRP:HE3	1:C:568:ILE:HD12	1.82	0.43
1:A:558:GLN:HE22	1:A:578:LYS:HB2	1.84	0.42
1:A:1673:PHE:O	1:A:1677:VAL:HG13	2.18	0.42
1:B:679:LEU:O	1:B:683:VAL:HG22	2.19	0.42
1:B:1023:LYS:HD3	1:B:1023:LYS:HA	1.82	0.42
1:C:1307:LYS:HA	1:C:1307:LYS:HD3	1.81	0.42
1:C:1721:HIS:HA	1:C:1724:TYR:CD1	2.53	0.42
1:C:2271:PHE:O	1:C:2274:ILE:HG22	2.19	0.42
1:A:2271:PHE:O	1:A:2274:ILE:HG22	2.19	0.42
1:B:217:ASN:O	1:B:221:THR:HG23	2.19	0.42
1:B:1154:GLN:NE2	1:B:1245:TYR:OH	2.52	0.42
1:C:511:TRP:NE1	1:C:586:LYS:HD2	2.34	0.42
1:C:1155:ARG:HH22	1:C:1197:GLN:CD	2.26	0.42
1:C:2532:LYS:HB2	1:C:2566:VAL:CG2	2.49	0.42
1:A:571:VAL:HG11	1:A:574:PHE:HB2	2.00	0.42
1:A:1962:ASP:N	1:A:1962:ASP:OD1	2.49	0.42
1:B:9:LEU:HD23	1:B:9:LEU:H	1.84	0.42
1:B:1363:TRP:O	1:B:1367:ILE:HG12	2.19	0.42
1:B:2764:HIS:HA	1:C:2768:PHE:CE2	2.54	0.42
1:C:1435:CYS:O	1:C:1439:LEU:HD13	2.19	0.42
1:C:1721:HIS:HA	1:C:1724:TYR:CE1	2.54	0.42
1:A:774:LYS:HD3	1:A:776:GLU:H	1.84	0.42
1:B:977:LEU:O	1:B:978:PHE:HB2	2.20	0.42
1:B:1690:GLU:OE1	1:B:1690:GLU:N	2.50	0.42
1:C:9:LEU:HD23	1:C:9:LEU:H	1.84	0.42
1:C:1094:GLN:O	1:C:1098:ARG:HG2	2.20	0.42
1:C:1109:LYS:H	1:C:1109:LYS:HG2	1.66	0.42
1:C:1363:TRP:O	1:C:1367:ILE:HG12	2.19	0.42
1:A:762:ASN:OD1	1:A:762:ASN:N	2.53	0.42
1:A:1307:LYS:HD3	1:A:1307:LYS:HA	1.81	0.42
1:A:1686:SER:HA	1:A:1689:ARG:HG3	2.02	0.42
1:B:2532:LYS:HB2	1:B:2566:VAL:CG2	2.49	0.42
1:C:691:TRP:HD1	1:C:808:HIS:ND1	2.18	0.42
1:C:1297:ILE:HD13	1:C:1457:ASP:HB2	1.99	0.42
1:A:2532:LYS:HB2	1:A:2566:VAL:CG2	2.49	0.42
1:C:558:GLN:HE22	1:C:578:LYS:HB2	1.85	0.42
1:C:568:ILE:HD11	1:C:577:LYS:HD3	2.02	0.42
1:C:1023:LYS:HD3	1:C:1023:LYS:HA	1.82	0.42
1:C:1686:SER:HA	1:C:1689:ARG:HG3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:ILE:O	1:A:591:ILE:HG23	2.20	0.42
1:A:1266:ALA:HA	1:A:1269:ARG:HB3	2.02	0.42
1:A:2313:THR:HA	1:A:2316:VAL:HG12	2.01	0.42
1:B:568:ILE:HD11	1:B:577:LYS:HD3	2.02	0.42
1:B:2527:GLN:O	1:B:2528:GLN:HG2	2.19	0.42
1:A:568:ILE:HD11	1:A:577:LYS:HD3	2.02	0.42
1:A:691:TRP:HD1	1:A:808:HIS:ND1	2.18	0.42
1:A:1690:GLU:OE1	1:A:1690:GLU:N	2.50	0.42
1:A:1721:HIS:HA	1:A:1724:TYR:CE1	2.54	0.42
1:B:1686:SER:HA	1:B:1689:ARG:HG3	2.02	0.42
1:B:2344:MET:HE3	1:B:2344:MET:HB3	1.91	0.42
1:B:2587:MET:O	1:B:2590:GLU:HG2	2.19	0.42
1:C:2527:GLN:O	1:C:2528:GLN:HG2	2.19	0.42
1:A:1200:VAL:HG13	1:A:1232:PRO:HD3	2.02	0.42
1:A:2521:ILE:HA	1:A:2577:TRP:CD1	2.55	0.42
1:B:511:TRP:NE1	1:B:586:LYS:HD2	2.34	0.42
1:B:691:TRP:HD1	1:B:808:HIS:ND1	2.18	0.42
1:B:735:LYS:HE3	1:B:735:LYS:HB3	1.91	0.42
1:B:1094:GLN:O	1:B:1098:ARG:HG2	2.20	0.42
1:B:1351:LEU:HD23	1:B:1351:LEU:HA	1.85	0.42
1:B:1986:ASN:HA	1:B:1989:VAL:HG12	2.02	0.42
1:C:587:ILE:O	1:C:591:ILE:HG23	2.20	0.42
1:C:2348:LEU:HD23	1:C:2353:GLU:HG2	2.02	0.42
1:C:2521:ILE:HA	1:C:2577:TRP:CD1	2.55	0.42
1:A:1094:GLN:O	1:A:1098:ARG:HG2	2.20	0.42
1:B:558:GLN:HE22	1:B:578:LYS:HB2	1.85	0.42
1:B:2313:THR:HA	1:B:2316:VAL:HG12	2.01	0.42
1:C:1986:ASN:HA	1:C:1989:VAL:HG12	2.02	0.42
1:A:1684:LEU:HD12	1:A:1987:THR:OG1	2.20	0.41
1:A:2430:LEU:HB3	1:A:2434:SER:HB2	2.02	0.41
1:B:75:ILE:HD12	1:B:75:ILE:HA	1.91	0.41
1:B:1669:THR:O	1:B:1672:LEU:HG	2.20	0.41
1:B:2507:LEU:HD13	1:B:2609:ASN:H	1.85	0.41
1:C:1440:LEU:HD23	1:C:1440:LEU:HA	1.88	0.41
1:C:1669:THR:O	1:C:1672:LEU:HG	2.20	0.41
1:C:2587:MET:O	1:C:2590:GLU:HG2	2.19	0.41
1:A:977:LEU:O	1:A:978:PHE:HB2	2.20	0.41
1:A:1957:LYS:HB3	1:A:1957:LYS:HE3	1.83	0.41
1:A:2527:GLN:O	1:A:2528:GLN:HG2	2.19	0.41
1:B:587:ILE:O	1:B:591:ILE:HG23	2.20	0.41
1:B:2580:SER:HB2	1:B:2582:PRO:HD2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:VAL:O	1:C:211:LEU:HG	2.20	0.41
1:C:774:LYS:HD3	1:C:776:GLU:H	1.85	0.41
1:C:977:LEU:O	1:C:978:PHE:HB2	2.20	0.41
1:C:2580:SER:HB2	1:C:2582:PRO:HD2	2.02	0.41
1:A:511:TRP:NE1	1:A:586:LYS:HD2	2.34	0.41
1:A:2507:LEU:HD13	1:A:2609:ASN:H	1.85	0.41
1:A:2580:SER:HB2	1:A:2582:PRO:HD2	2.02	0.41
1:C:1351:LEU:HD23	1:C:1351:LEU:HA	1.85	0.41
1:C:1707:ARG:HD3	1:C:1959:PHE:HZ	1.85	0.41
1:C:2369:LYS:HD3	1:C:2369:LYS:HA	1.86	0.41
1:A:1041:ILE:HG22	1:A:1043:LEU:H	1.86	0.41
1:A:1280:MET:HE3	1:A:1357:LYS:HG3	2.03	0.41
1:A:1669:THR:O	1:A:1672:LEU:HG	2.20	0.41
1:A:1993:GLU:HG2	1:A:1997:TYR:CE2	2.55	0.41
1:A:2754:PHE:CZ	1:C:2753:LYS:NZ	2.62	0.41
1:B:37:TYR:O	1:B:41:ILE:HG13	2.20	0.41
1:B:774:LYS:HD3	1:B:776:GLU:H	1.85	0.41
1:B:2348:LEU:HD23	1:B:2353:GLU:HG2	2.02	0.41
1:B:2430:LEU:HB3	1:B:2434:SER:HB2	2.02	0.41
1:C:2587:MET:O	1:C:2591:LEU:HG	2.20	0.41
1:A:1674:LEU:HA	1:A:1677:VAL:HG22	2.03	0.41
1:A:2587:MET:O	1:A:2591:LEU:HG	2.20	0.41
1:B:1993:GLU:HG2	1:B:1997:TYR:CE2	2.55	0.41
1:C:752:LEU:HD21	1:C:798:PRO:HB2	2.03	0.41
1:C:762:ASN:OD1	1:C:762:ASN:N	2.53	0.41
1:C:786:PHE:HB3	1:C:790:GLU:HG3	2.03	0.41
1:C:1200:VAL:HG13	1:C:1232:PRO:HD3	2.02	0.41
1:C:1266:ALA:HA	1:C:1269:ARG:HB3	2.02	0.41
1:C:1466:SER:HG	1:C:1717:ARG:HE	1.65	0.41
1:C:2020:PHE:CZ	1:C:2370:CYS:HB3	2.54	0.41
1:A:207:VAL:O	1:A:211:LEU:HG	2.20	0.41
1:A:1986:ASN:HA	1:A:1989:VAL:HG12	2.02	0.41
1:A:2348:LEU:HD23	1:A:2353:GLU:HG2	2.02	0.41
1:A:2643:ASP:O	1:A:2644:THR:HG22	2.21	0.41
1:B:1718:GLU:O	1:B:1722:MET:HG2	2.21	0.41
1:B:2464:GLN:O	1:B:2465:LYS:HG2	2.21	0.41
1:C:511:TRP:CZ2	1:C:554:LEU:HD11	2.56	0.41
1:C:1684:LEU:HD12	1:C:1987:THR:OG1	2.20	0.41
1:C:2539:TYR:O	1:C:2543:LEU:HG	2.21	0.41
1:A:289:TYR:OH	1:A:294:PHE:O	2.39	0.41
1:A:1215:ARG:NH2	1:A:1223:ASP:OD1	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2464:GLN:O	1:A:2465:LYS:HG2	2.21	0.41
1:B:752:LEU:HD21	1:B:798:PRO:HB2	2.03	0.41
1:B:1211:ASP:OD1	1:B:1212:TYR:N	2.38	0.41
1:B:1266:ALA:HA	1:B:1269:ARG:HB3	2.02	0.41
1:C:37:TYR:O	1:C:41:ILE:HG13	2.20	0.41
1:C:815:ARG:HA	1:C:818:GLU:HG2	2.03	0.41
1:C:952:TRP:HZ3	1:C:1090:VAL:HA	1.85	0.41
1:C:1215:ARG:NH2	1:C:1223:ASP:OD1	2.54	0.41
1:A:588:LEU:HD12	1:A:591:ILE:HD11	2.03	0.41
1:A:815:ARG:HA	1:A:818:GLU:HG2	2.03	0.41
1:A:952:TRP:HZ3	1:A:1090:VAL:HA	1.85	0.41
1:A:1023:LYS:HA	1:A:1023:LYS:HD3	1.82	0.41
1:A:2759:PHE:CZ	1:B:2416:GLU:HB2	2.55	0.41
1:A:2804:ILE:HD13	1:A:2804:ILE:HA	1.94	0.41
1:B:256:TRP:HE1	1:B:262:THR:C	2.29	0.41
1:B:519:LEU:O	1:B:522:VAL:HG12	2.21	0.41
1:B:1684:LEU:HD12	1:B:1987:THR:OG1	2.20	0.41
1:B:2521:ILE:HA	1:B:2577:TRP:CD1	2.55	0.41
1:C:2313:THR:HA	1:C:2316:VAL:HG12	2.01	0.41
1:A:9:LEU:H	1:A:9:LEU:HD23	1.84	0.41
1:A:239:PRO:HG3	1:A:580:PRO:HB3	2.03	0.41
1:A:284:ILE:HD13	1:A:284:ILE:HA	1.97	0.41
1:A:519:LEU:O	1:A:522:VAL:HG12	2.21	0.41
1:A:555:LEU:HD12	1:A:555:LEU:HA	1.83	0.41
1:A:2261:VAL:HG13	1:A:2262:LEU:HD22	2.03	0.41
1:A:2488:PHE:N	1:A:2489:PRO:HD2	2.36	0.41
1:B:251:LEU:HD21	1:B:552:ASN:ND2	2.36	0.41
1:B:786:PHE:HB3	1:B:790:GLU:HG3	2.03	0.41
1:B:1041:ILE:HG22	1:B:1043:LEU:H	1.86	0.41
1:B:1159:TYR:O	1:B:1163:HIS:ND1	2.50	0.41
1:B:2546:PHE:CE2	1:B:2675:LEU:HD12	2.56	0.41
1:C:289:TYR:OH	1:C:294:PHE:O	2.39	0.41
1:C:977:LEU:C	1:C:979:ASN:H	2.29	0.41
1:C:1041:ILE:HG22	1:C:1043:LEU:H	1.86	0.41
1:C:1280:MET:HE3	1:C:1357:LYS:HG3	2.03	0.41
1:C:1674:LEU:HA	1:C:1677:VAL:HG22	2.03	0.41
1:C:1718:GLU:O	1:C:1722:MET:HG2	2.21	0.41
1:C:1993:GLU:HG2	1:C:1997:TYR:CE2	2.55	0.41
1:C:2488:PHE:N	1:C:2489:PRO:HD2	2.36	0.41
1:A:251:LEU:HD21	1:A:552:ASN:ND2	2.36	0.41
1:A:1117:ARG:HB2	1:A:1272:ALA:HA	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2310:GLN:O	1:A:2313:THR:HG22	2.21	0.41
1:A:2416:GLU:HB2	1:C:2759:PHE:CZ	2.55	0.41
1:A:2541:GLU:HG3	1:A:2544:LYS:HE2	2.03	0.41
1:A:2546:PHE:CE2	1:A:2675:LEU:HD12	2.56	0.41
1:B:2310:GLN:O	1:B:2313:THR:HG22	2.21	0.41
1:C:1131:PHE:O	1:C:1135:PHE:HB2	2.21	0.41
1:C:1360:LEU:HD23	1:C:1360:LEU:HA	1.87	0.41
1:C:1484:ILE:HG13	1:C:1485:GLU:N	2.36	0.41
1:C:1964:LEU:O	1:C:1968:GLU:HG2	2.21	0.41
1:C:2507:LEU:HD13	1:C:2609:ASN:H	1.85	0.41
1:C:2541:GLU:HG3	1:C:2544:LYS:HE2	2.03	0.41
1:A:1466:SER:HG	1:A:1717:ARG:HE	1.68	0.40
1:A:2539:TYR:O	1:A:2543:LEU:HG	2.21	0.40
1:B:732:TRP:O	1:B:736:ILE:HG12	2.21	0.40
1:B:957:LEU:HD12	1:B:957:LEU:HA	1.94	0.40
1:B:1200:VAL:HG13	1:B:1232:PRO:HD3	2.02	0.40
1:B:1215:ARG:NH2	1:B:1223:ASP:OD1	2.54	0.40
1:B:2556:LEU:HD23	1:B:2675:LEU:HD11	2.03	0.40
1:C:2430:LEU:HB3	1:C:2434:SER:HB2	2.02	0.40
1:C:2464:GLN:O	1:C:2465:LYS:HG2	2.21	0.40
1:A:37:TYR:O	1:A:41:ILE:HG13	2.20	0.40
1:A:245:VAL:O	1:A:249:VAL:HG12	2.21	0.40
1:A:1707:ARG:HD3	1:A:1959:PHE:HZ	1.85	0.40
1:B:511:TRP:CZ2	1:B:554:LEU:HD11	2.56	0.40
1:B:815:ARG:HA	1:B:818:GLU:HG2	2.03	0.40
1:B:1964:LEU:O	1:B:1968:GLU:HG2	2.21	0.40
1:B:2566:VAL:HG12	1:B:2721:VAL:HG13	2.04	0.40
1:B:2586:LYS:HE3	1:C:2570:GLU:OE2	2.22	0.40
1:B:2587:MET:O	1:B:2591:LEU:HG	2.21	0.40
1:C:705:GLU:O	1:C:712:LYS:NZ	2.43	0.40
1:C:732:TRP:O	1:C:736:ILE:HG12	2.21	0.40
1:C:1709:ILE:HD12	1:C:1709:ILE:HA	1.89	0.40
1:C:2765:SER:O	1:C:2765:SER:OG	2.38	0.40
1:A:261:ARG:HD2	1:A:261:ARG:HA	1.91	0.40
1:A:732:TRP:O	1:A:736:ILE:HG12	2.21	0.40
1:A:1131:PHE:O	1:A:1135:PHE:HB2	2.22	0.40
1:A:1718:GLU:O	1:A:1722:MET:HG2	2.21	0.40
1:A:2553:MET:O	1:A:2556:LEU:HG	2.21	0.40
1:A:2566:VAL:HG12	1:A:2721:VAL:HG13	2.03	0.40
1:B:286:LEU:HD23	1:B:286:LEU:HA	1.95	0.40
1:B:1230:TYR:OH	1:B:1239:ASN:O	2.35	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2541:GLU:HG3	1:B:2544:LYS:HE2	2.03	0.40
1:C:2395:LYS:HE2	1:C:2395:LYS:HB3	1.89	0.40
1:B:207:VAL:O	1:B:211:LEU:HG	2.20	0.40
1:B:1707:ARG:HD3	1:B:1959:PHE:HZ	1.85	0.40
1:B:2237:ILE:HD12	1:B:2237:ILE:HA	1.95	0.40
1:B:2710:ILE:HG22	1:B:2711:PHE:N	2.35	0.40
1:C:239:PRO:HG3	1:C:580:PRO:HB3	2.03	0.40
1:C:1711:LYS:HE3	1:C:1711:LYS:HB3	1.94	0.40
1:C:2556:LEU:HD23	1:C:2675:LEU:HD11	2.04	0.40
1:C:2643:ASP:O	1:C:2644:THR:HG22	2.21	0.40
1:A:511:TRP:CZ2	1:A:554:LEU:HD11	2.56	0.40
1:A:2461:PRO:HD2	1:A:2464:GLN:NE2	2.31	0.40
1:B:239:PRO:HG3	1:B:580:PRO:HB3	2.03	0.40
1:B:1157:ASP:HB2	1:B:1228:TRP:O	2.21	0.40
1:B:2261:VAL:HG13	1:B:2262:LEU:HD22	2.03	0.40
1:B:2488:PHE:N	1:B:2489:PRO:HD2	2.36	0.40
1:B:2643:ASP:O	1:B:2644:THR:HG22	2.21	0.40
1:B:2759:PHE:CZ	1:C:2416:GLU:HB2	2.56	0.40
1:C:519:LEU:O	1:C:522:VAL:HG12	2.21	0.40
1:C:588:LEU:HD12	1:C:591:ILE:HD11	2.03	0.40
1:C:2344:MET:HE3	1:C:2344:MET:HB3	1.91	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	1786/2822 (63%)	1683 (94%)	103 (6%)	0	100	100
1	B	1786/2822 (63%)	1684 (94%)	102 (6%)	0	100	100
1	C	1786/2822 (63%)	1684 (94%)	102 (6%)	0	100	100
All	All	5358/8466 (63%)	5051 (94%)	307 (6%)	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	1626/2541 (64%)	1626 (100%)	0	100	100
1	B	1561/2541 (61%)	1561 (100%)	0	100	100
1	C	1626/2541 (64%)	1626 (100%)	0	100	100
All	All	4813/7623 (63%)	4813 (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 (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	61	GLN
1	A	292	GLN
1	A	357	GLN
1	A	558	GLN
1	A	600	HIS
1	A	729	HIS
1	A	785	GLN
1	A	979	ASN
1	A	1018	GLN
1	A	1076	ASN
1	A	1094	GLN
1	A	1154	GLN
1	A	1370	ASN
1	A	1442	GLN
1	A	1721	HIS
1	A	1727	HIS
1	A	2053	GLN
1	A	2310	GLN
1	A	2444	HIS
1	A	2460	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2519	GLN
1	A	2528	GLN
1	A	2607	GLN
1	A	2609	ASN
1	A	2674	GLN
1	A	2713	GLN
1	B	53	GLN
1	B	61	GLN
1	B	292	GLN
1	B	357	GLN
1	B	552	ASN
1	B	558	GLN
1	B	600	HIS
1	B	785	GLN
1	B	979	ASN
1	B	1018	GLN
1	B	1026	ASN
1	B	1076	ASN
1	B	1094	GLN
1	B	1154	GLN
1	B	1370	ASN
1	B	1442	GLN
1	B	1721	HIS
1	B	1727	HIS
1	B	2053	GLN
1	B	2310	GLN
1	B	2444	HIS
1	B	2460	GLN
1	B	2519	GLN
1	B	2528	GLN
1	B	2607	GLN
1	B	2609	ASN
1	B	2674	GLN
1	B	2713	GLN
1	C	53	GLN
1	C	61	GLN
1	C	292	GLN
1	C	357	GLN
1	C	558	GLN
1	C	600	HIS
1	C	729	HIS
1	C	785	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	979	ASN
1	C	1018	GLN
1	C	1076	ASN
1	C	1094	GLN
1	C	1154	GLN
1	C	1370	ASN
1	C	1442	GLN
1	C	1727	HIS
1	C	2053	GLN
1	C	2310	GLN
1	C	2444	HIS
1	C	2460	GLN
1	C	2519	GLN
1	C	2528	GLN
1	C	2607	GLN
1	C	2609	ASN
1	C	2674	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](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	3002	1	14,14,15	1.29	2 (14%)	17,19,21	0.82	0
2	NAG	A	3003	1	14,14,15	1.30	2 (14%)	17,19,21	0.68	0
2	NAG	B	3004	1	14,14,15	1.31	2 (14%)	17,19,21	0.58	0
2	NAG	B	3001	1	14,14,15	0.34	0	17,19,21	0.72	1 (5%)
2	NAG	C	3003	1	14,14,15	1.29	2 (14%)	17,19,21	0.68	0
2	NAG	B	3003	1	14,14,15	1.30	2 (14%)	17,19,21	0.68	0
2	NAG	A	3004	1	14,14,15	1.32	2 (14%)	17,19,21	0.58	0
2	NAG	C	3002	1	14,14,15	1.29	2 (14%)	17,19,21	0.82	0
2	NAG	C	3004	1	14,14,15	1.32	2 (14%)	17,19,21	0.58	0
2	NAG	C	3001	1	14,14,15	0.33	0	17,19,21	0.72	1 (5%)
2	NAG	B	3002	1	14,14,15	1.30	2 (14%)	17,19,21	0.82	0
2	NAG	A	3001	1	14,14,15	0.33	0	17,19,21	0.73	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	3002	1	-	5/6/23/26	0/1/1/1
2	NAG	A	3003	1	-	3/6/23/26	0/1/1/1
2	NAG	B	3004	1	-	2/6/23/26	0/1/1/1
2	NAG	B	3001	1	-	4/6/23/26	0/1/1/1
2	NAG	C	3003	1	-	3/6/23/26	0/1/1/1
2	NAG	B	3003	1	-	3/6/23/26	0/1/1/1
2	NAG	A	3004	1	-	2/6/23/26	0/1/1/1
2	NAG	C	3002	1	-	5/6/23/26	0/1/1/1
2	NAG	C	3004	1	-	2/6/23/26	0/1/1/1
2	NAG	C	3001	1	-	4/6/23/26	0/1/1/1
2	NAG	B	3002	1	-	5/6/23/26	0/1/1/1
2	NAG	A	3001	1	-	4/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3004	NAG	O5-C1	4.27	1.50	1.43
2	C	3004	NAG	O5-C1	4.26	1.50	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3004	NAG	O5-C1	4.25	1.50	1.43
2	B	3003	NAG	O5-C1	4.16	1.50	1.43
2	B	3002	NAG	O5-C1	4.15	1.50	1.43
2	C	3003	NAG	O5-C1	4.13	1.50	1.43
2	A	3003	NAG	O5-C1	4.13	1.50	1.43
2	A	3002	NAG	O5-C1	4.12	1.50	1.43
2	C	3002	NAG	O5-C1	4.10	1.50	1.43
2	A	3003	NAG	O5-C5	2.30	1.47	1.43
2	C	3002	NAG	O5-C5	2.28	1.47	1.43
2	C	3003	NAG	O5-C5	2.27	1.47	1.43
2	B	3003	NAG	O5-C5	2.27	1.47	1.43
2	A	3002	NAG	O5-C5	2.26	1.47	1.43
2	B	3002	NAG	O5-C5	2.26	1.47	1.43
2	C	3004	NAG	O5-C5	2.19	1.47	1.43
2	A	3004	NAG	O5-C5	2.17	1.47	1.43
2	B	3004	NAG	O5-C5	2.16	1.47	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001	NAG	C1-O5-C5	2.14	115.06	112.19
2	C	3001	NAG	C1-O5-C5	2.12	115.03	112.19
2	B	3001	NAG	C1-O5-C5	2.11	115.02	112.19

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3002	NAG	C1-C2-N2-C7
2	A	3002	NAG	C8-C7-N2-C2
2	A	3003	NAG	C1-C2-N2-C7
2	B	3002	NAG	C1-C2-N2-C7
2	B	3002	NAG	C8-C7-N2-C2
2	B	3003	NAG	C1-C2-N2-C7
2	C	3002	NAG	C1-C2-N2-C7
2	C	3002	NAG	C8-C7-N2-C2
2	C	3003	NAG	C1-C2-N2-C7
2	A	3002	NAG	O5-C5-C6-O6
2	B	3002	NAG	O5-C5-C6-O6
2	C	3002	NAG	O5-C5-C6-O6
2	A	3002	NAG	O7-C7-N2-C2
2	B	3002	NAG	O7-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	3002	NAG	O7-C7-N2-C2
2	A	3004	NAG	C4-C5-C6-O6
2	B	3004	NAG	C4-C5-C6-O6
2	C	3004	NAG	C4-C5-C6-O6
2	A	3002	NAG	C4-C5-C6-O6
2	B	3002	NAG	C4-C5-C6-O6
2	C	3002	NAG	C4-C5-C6-O6
2	A	3004	NAG	O5-C5-C6-O6
2	B	3004	NAG	O5-C5-C6-O6
2	C	3004	NAG	O5-C5-C6-O6
2	A	3001	NAG	C8-C7-N2-C2
2	B	3001	NAG	C8-C7-N2-C2
2	C	3001	NAG	C8-C7-N2-C2
2	A	3001	NAG	O7-C7-N2-C2
2	B	3001	NAG	O7-C7-N2-C2
2	C	3001	NAG	O7-C7-N2-C2
2	A	3003	NAG	C4-C5-C6-O6
2	B	3003	NAG	C4-C5-C6-O6
2	C	3003	NAG	C4-C5-C6-O6
2	A	3003	NAG	O5-C5-C6-O6
2	B	3003	NAG	O5-C5-C6-O6
2	C	3003	NAG	O5-C5-C6-O6
2	A	3001	NAG	O5-C5-C6-O6
2	B	3001	NAG	O5-C5-C6-O6
2	C	3001	NAG	O5-C5-C6-O6
2	A	3001	NAG	C1-C2-N2-C7
2	B	3001	NAG	C1-C2-N2-C7
2	C	3001	NAG	C1-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3002	NAG	4	0
2	A	3003	NAG	1	0
2	C	3003	NAG	1	0
2	B	3003	NAG	1	0
2	C	3002	NAG	4	0
2	B	3002	NAG	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

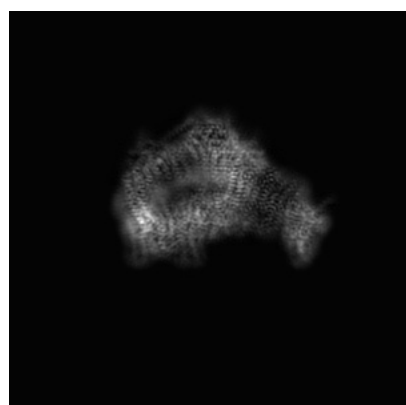
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9975. These allow visual inspection of the internal detail of the map and identification of artifacts.

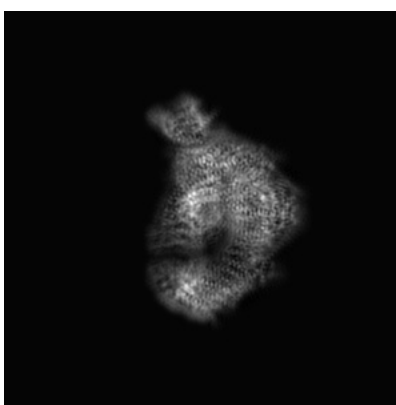
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

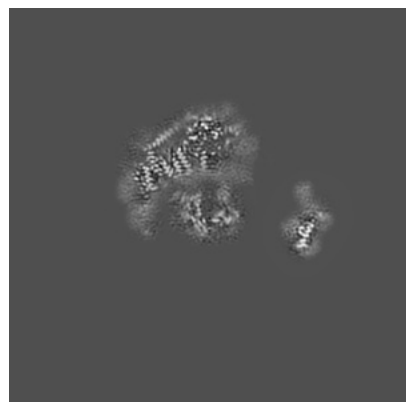


Z

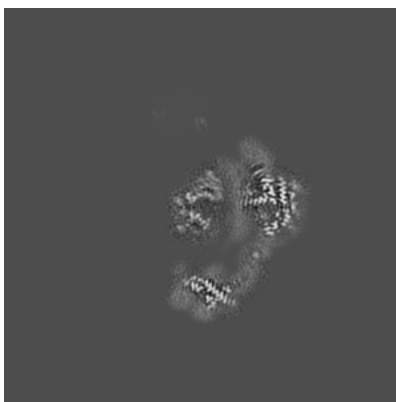
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

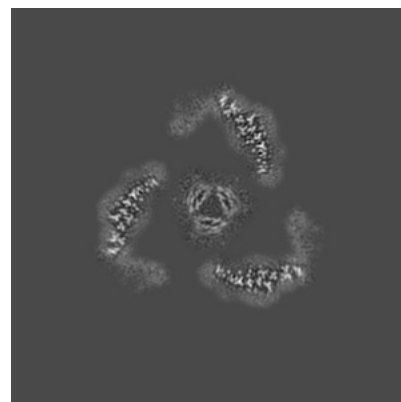
6.2.1 Primary map



X Index: 160



Y Index: 160

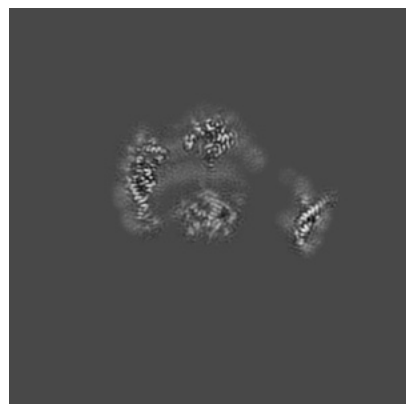


Z Index: 160

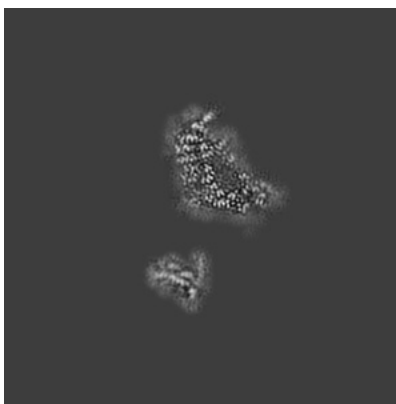
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

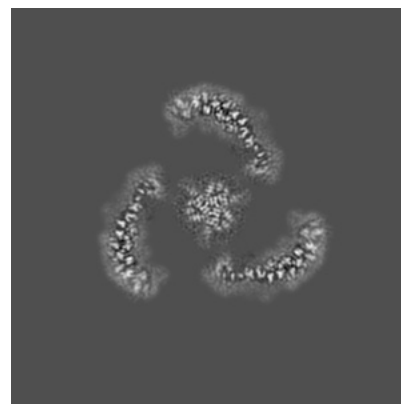
6.3.1 Primary map



X Index: 168



Y Index: 107

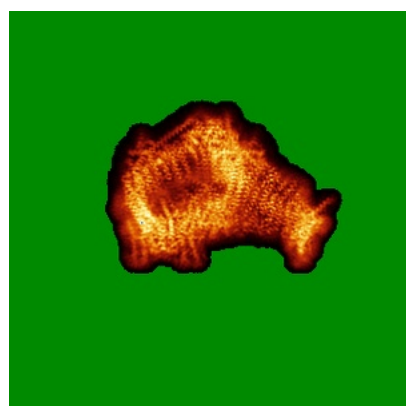


Z Index: 150

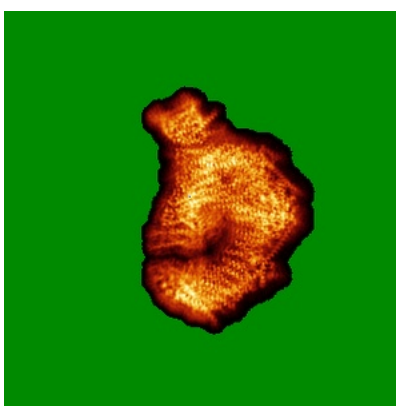
The images above show the largest variance slices of the map in three orthogonal directions.

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

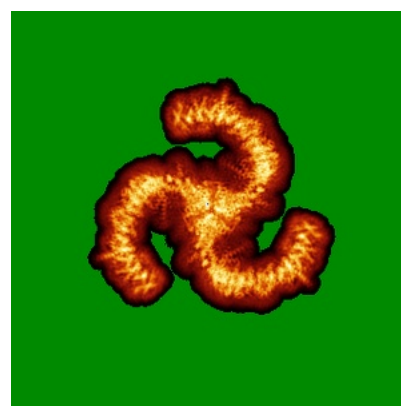
6.4.1 Primary map



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

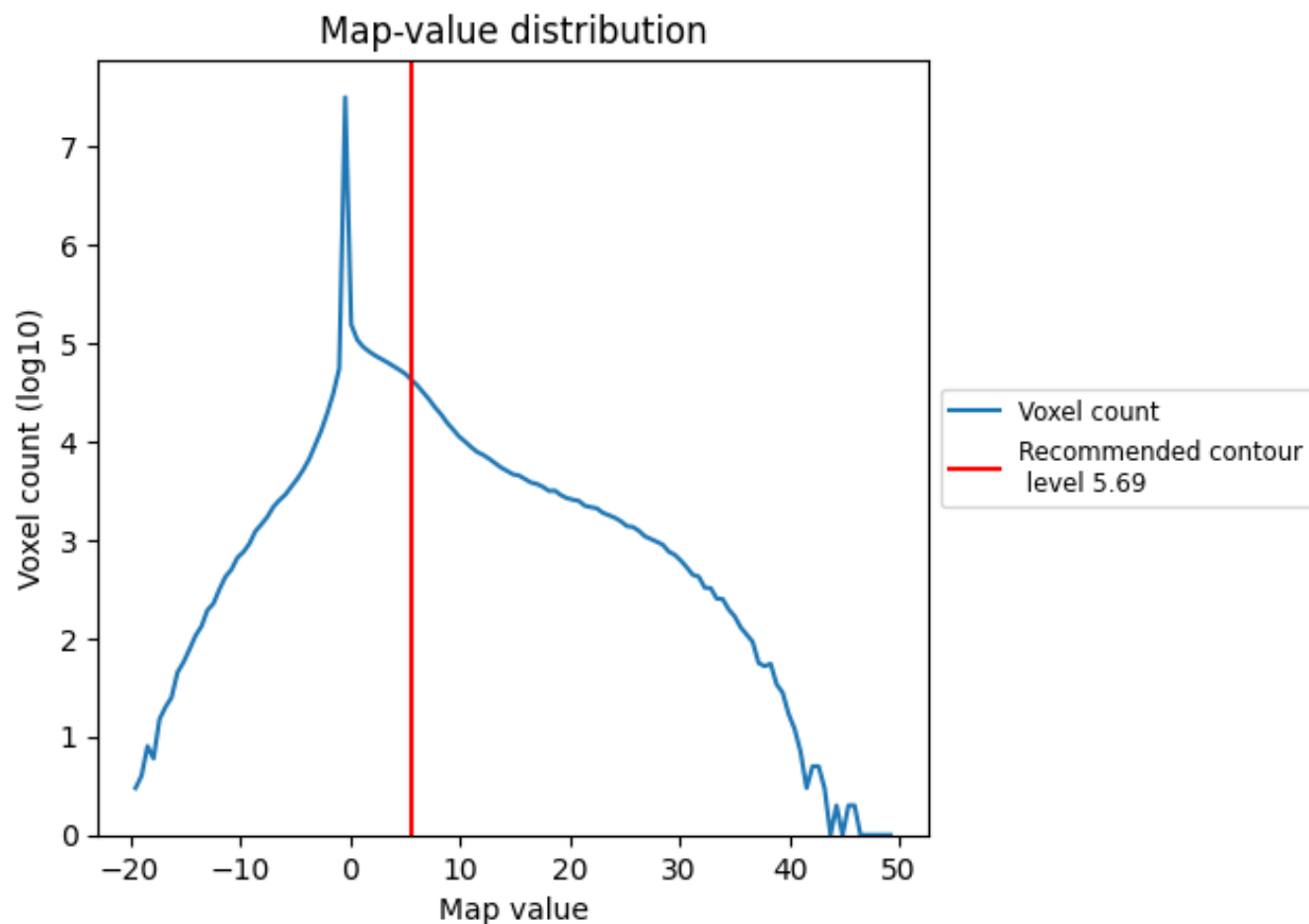
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

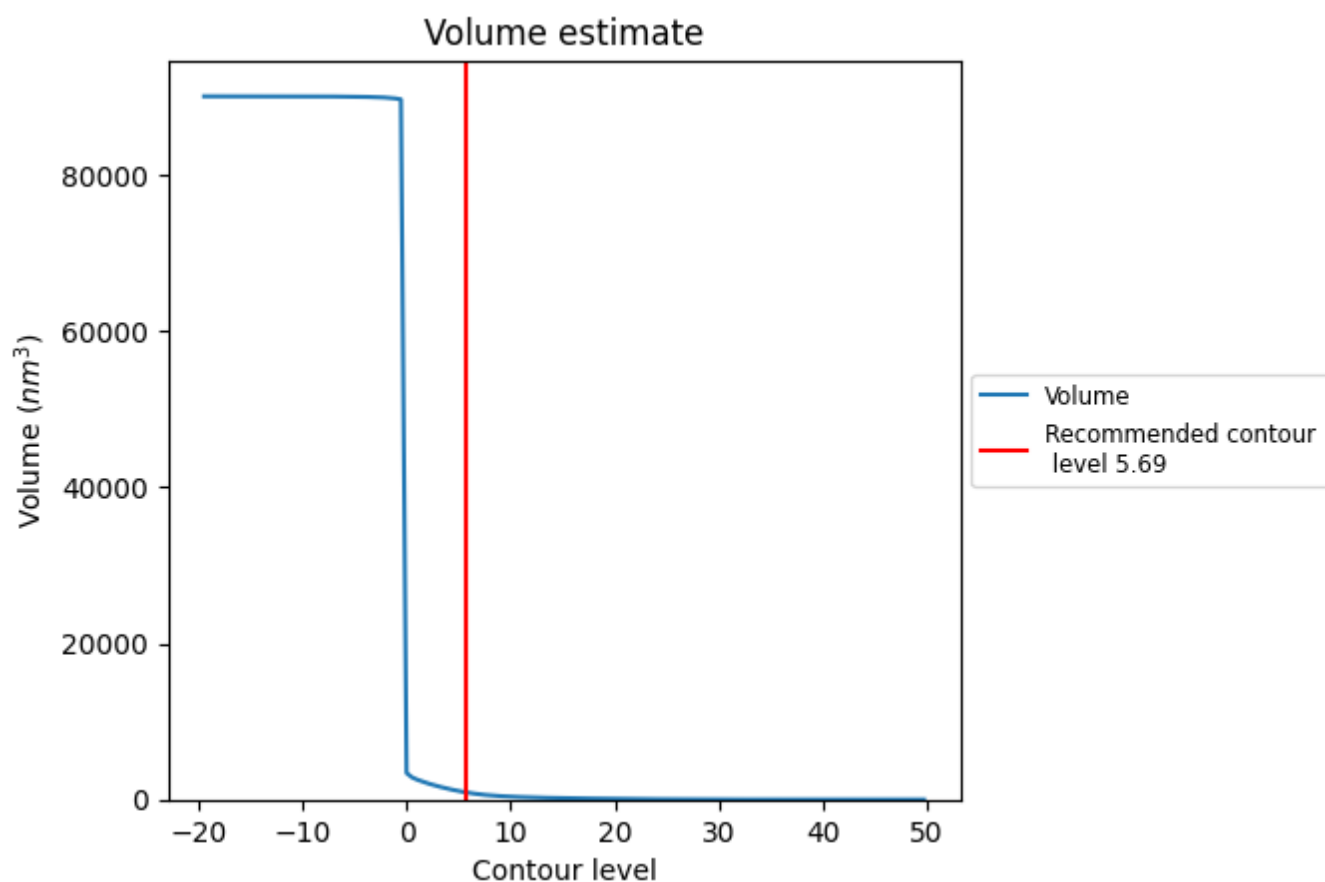
This section contains the results of statistical analysis of the map.

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.

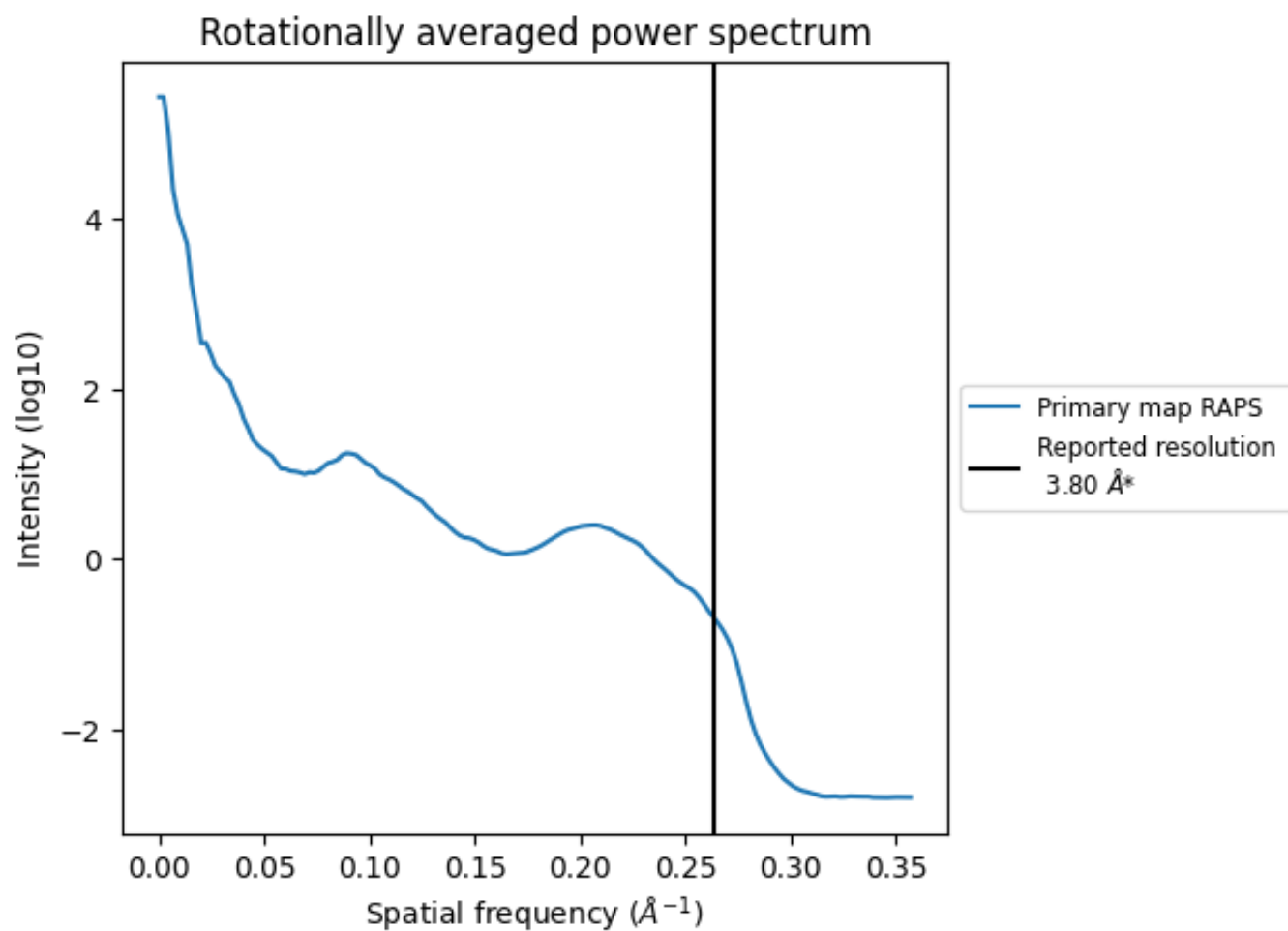
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 925 nm^3 ; this corresponds to an approximate mass of 836 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 0.263 Å⁻¹

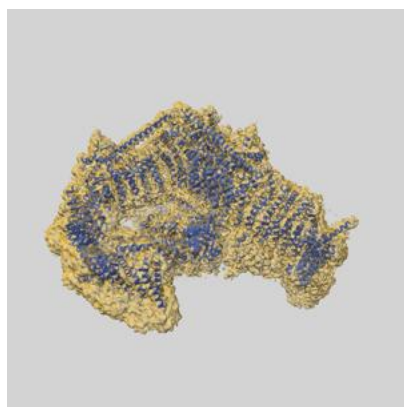
8 Fourier-Shell correlation

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

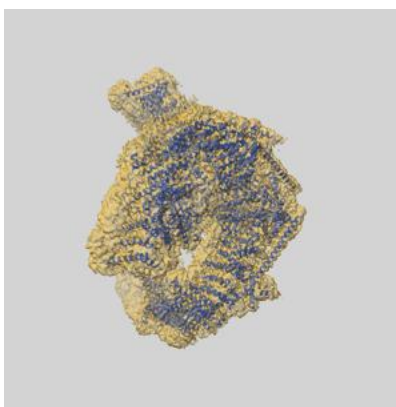
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9975 and PDB model 6KG7. Per-residue inclusion information can be found in section 3 on page 5.

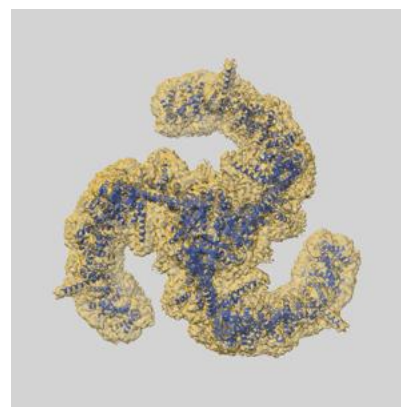
9.1 Map-model overlay [i](#)



X



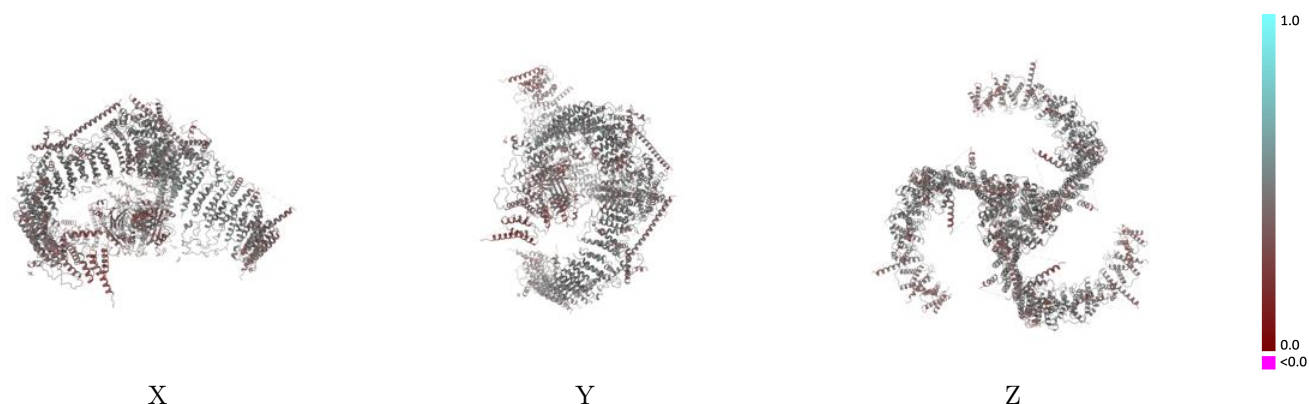
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.69 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](#)

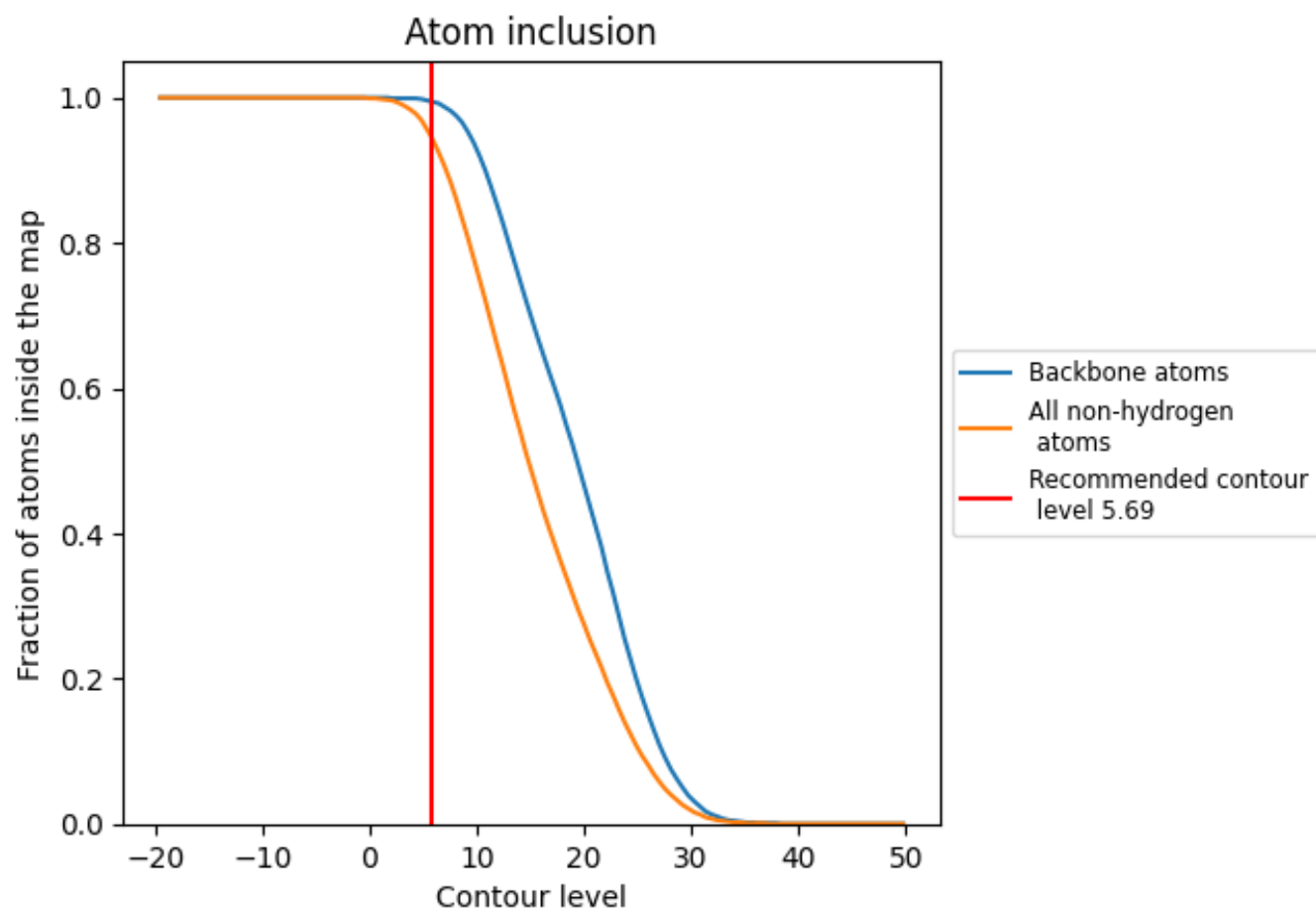


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 100% of all backbone atoms, 95% 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 (5.69) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9480	0.4370
A	0.9460	0.4410
B	0.9490	0.4370
C	0.9480	0.4320

