



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 01:51 PM UTC

PDB ID : 7Z12 / pdb_00007z12
EMDB ID : EMD-14438
Title : VAR2 complex with PAM1.4
Authors : Raghavan, S.S.R.; Wang, K.T.
Deposited on : 2022-02-24
Resolution : 3.00 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:

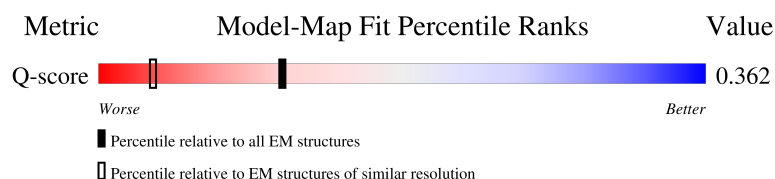
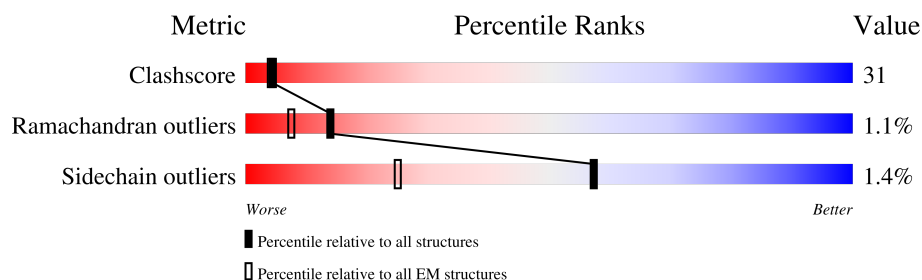
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.00 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	14081 (2.50 - 3.50)

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	B	472	 30% 17% 53%
2	C	233	 55% 36% 9%
3	A	2040	 20% 43% 44% .. 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18352 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 PAM1.4, Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	221	Total	C	N	O	S	0	0
			1650	1042	283	319	6		

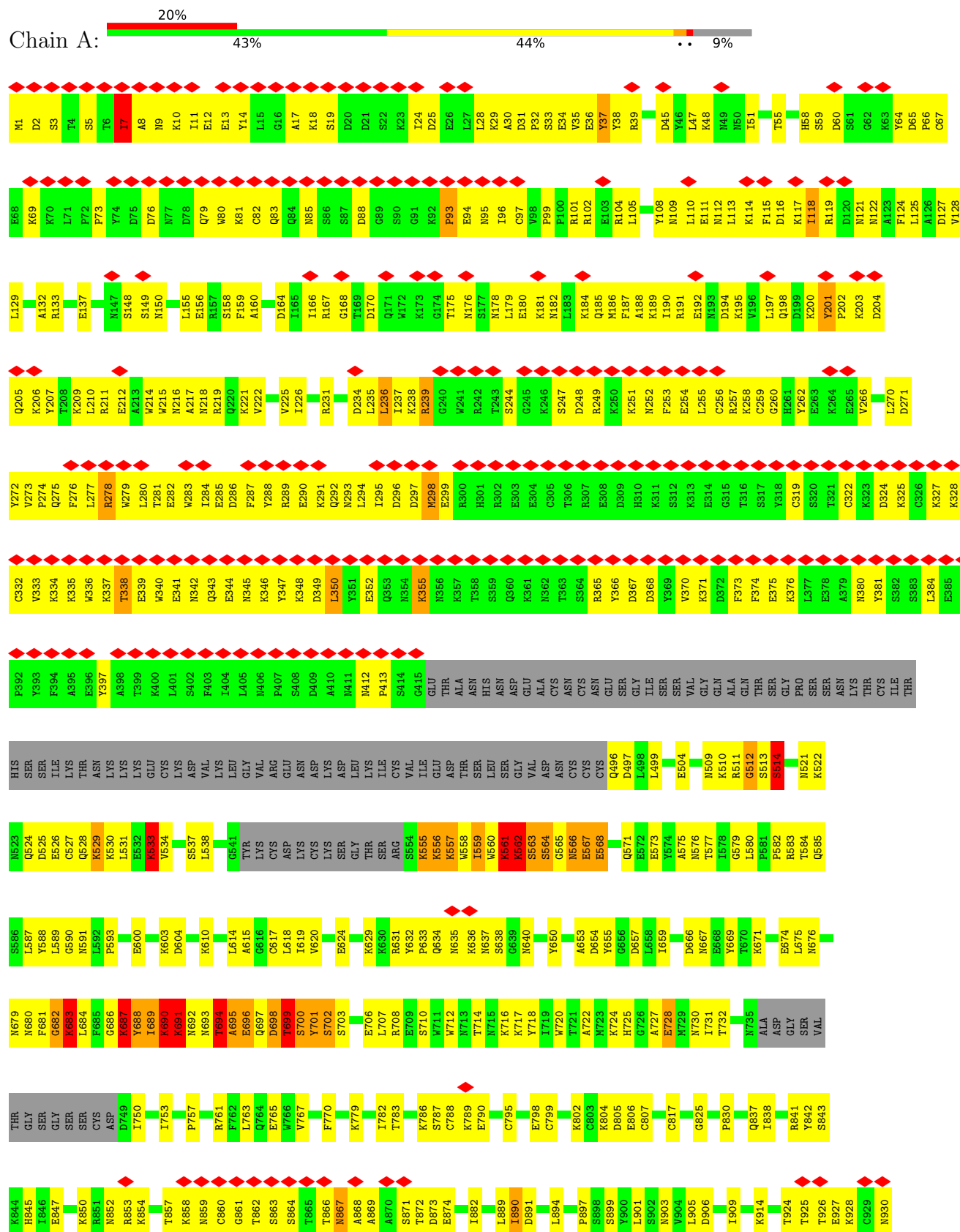
- Molecule 2 is a protein called PAM1.4, light Chain.

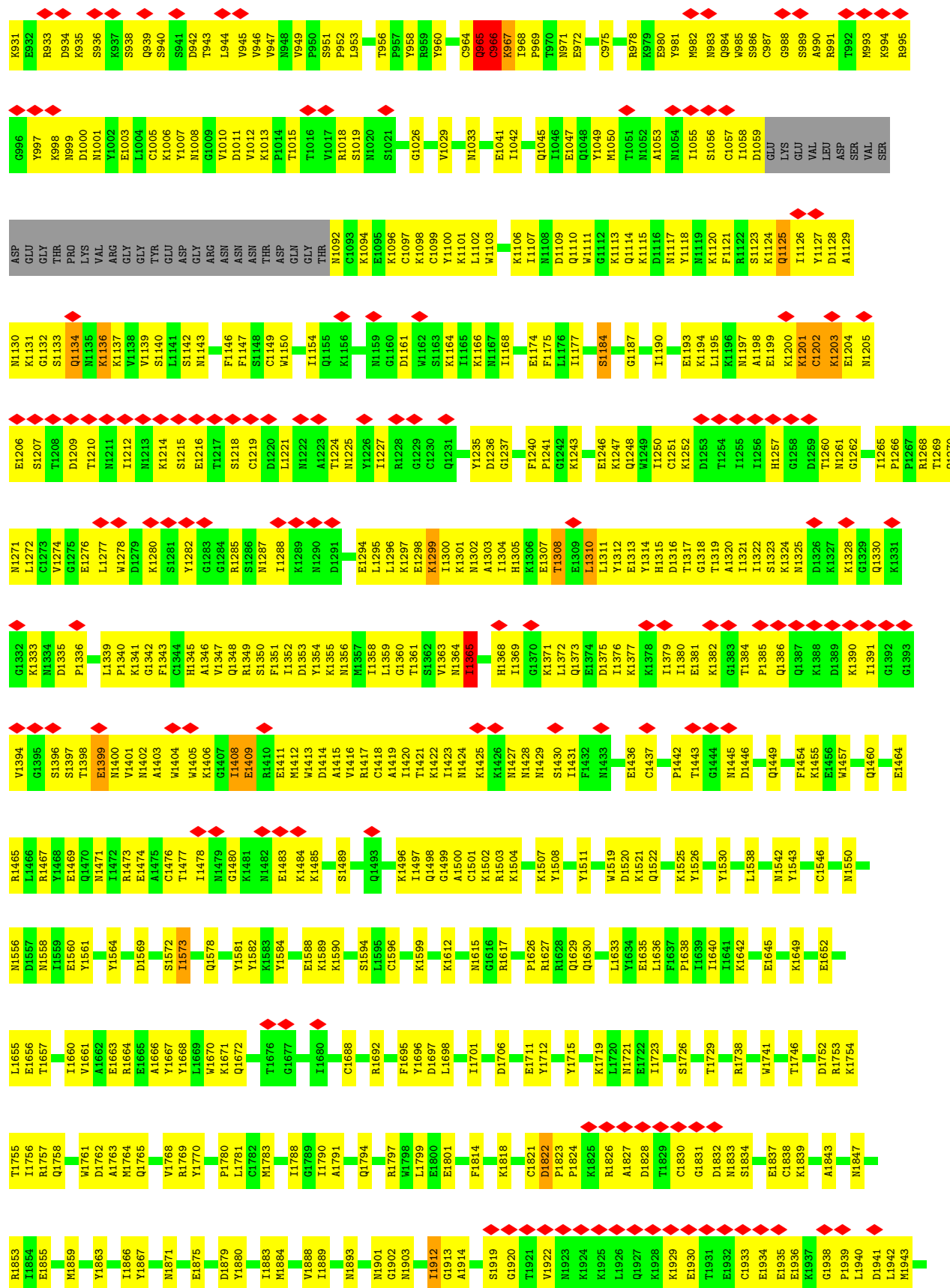
Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	212	Total	C	N	O	S	0	0
			1631	1021	279	326	5		

- Molecule 3 is a protein called VAR2CSA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1853	Total	C	N	O	S	0	0
			15071	9402	2597	2973	99		

● Molecule 3: VAR2CSA





LYS	ASP	LYS	THR	LYS	LEU	ASP	GLU	LEU	ASP	GLU	ASP	TRP	ASN	ASP	MET	ASP	LEU	ARG	GLY	THR	TYR	ASN	LYS	HIS	LYS	GLY	VAL	LEU	ILE	PRO																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
Y1946	M1950	K1951	K1952	K1953	Y1954		H1957	K1958	M1959	K1960	C1961	T1962	E1963	V1964	Y1965	L1966	E1967	H1968	V1969		Q1972	L1973		I1976	D1977	N1978	A1979	I1980	K1981	D1982	Y1983	K1984	L1985	Y1986	P1987	L1988	D1989	R1990																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50000	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.352	Depositor
Minimum map value	-0.906	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	366.08002, 366.08002, 366.08002	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	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	B	0.29	0/1688	0.47	0/2297
2	C	0.27	0/1665	0.45	0/2263
3	A	0.34	0/15370	0.67	15/20668 (0.1%)
All	All	0.33	0/18723	0.64	15/25228 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
3	A	0	31
All	All	0	32

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1203	LYS	N-CA-C	7.88	127.59	110.80
3	A	562	LYS	CB-CA-C	-7.25	95.99	110.42
3	A	694	THR	CB-CA-C	-7.08	106.54	115.89
3	A	7	ILE	N-CA-C	-6.92	106.56	113.20
3	A	701	TYR	CB-CA-C	6.75	119.97	109.84
3	A	561	LYS	CA-C-N	-6.29	109.52	121.54
3	A	561	LYS	C-N-CA	-6.29	109.52	121.54
3	A	681	PHE	N-CA-C	-5.58	106.18	112.87
3	A	965	GLN	CA-C-N	5.43	131.90	121.54
3	A	965	GLN	C-N-CA	5.43	131.90	121.54
3	A	1573	ILE	N-CA-C	-5.35	107.50	112.43
3	A	1203	LYS	CA-C-N	5.31	131.25	121.70
3	A	1203	LYS	C-N-CA	5.31	131.25	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1310	LEU	CA-C-N	-5.06	113.97	120.65
3	A	1310	LEU	C-N-CA	-5.06	113.97	120.65

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	1125	GLN	Peptide
3	A	1134	GLN	Peptide
3	A	1136	LYS	Peptide
3	A	1184	SER	Peptide
3	A	1201	LYS	Peptide
3	A	1202	CYS	Peptide
3	A	1299	LYS	Peptide
3	A	1308	THR	Peptide
3	A	1365	ILE	Peptide
3	A	1399	GLU	Peptide
3	A	1403	ALA	Peptide
3	A	1408	ILE	Peptide
3	A	1409	GLU	Peptide
3	A	1822	ASP	Peptide
3	A	201	TYR	Peptide
3	A	236	LEU	Peptide
3	A	239	ARG	Peptide
3	A	278	ARG	Peptide
3	A	298	MET	Peptide
3	A	338	THR	Peptide
3	A	349	ASP	Peptide
3	A	355	LYS	Peptide
3	A	37	TYR	Peptide
3	A	529	LYS	Peptide
3	A	533	LYS	Peptide
3	A	698	ASP	Peptide
3	A	728	GLU	Peptide
3	A	786	LYS	Peptide
3	A	952	PRO	Peptide
3	A	965	GLN	Peptide
3	A	966	CYS	Peptide
2	C	48	ILE	Peptide

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	B	1650	0	1628	61	0
2	C	1631	0	1599	65	0
3	A	15071	0	14624	1014	0
All	All	18352	0	17851	1130	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 31.

All (1130) 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)
3:A:924:THR:HA	3:A:946:VAL:O	1.27	1.31
3:A:251:LYS:HB3	3:A:566:ASN:HB2	1.21	1.12
3:A:325:LYS:O	3:A:329:TYR:HB2	1.60	0.99
3:A:1050:MET:HE3	3:A:1198:ALA:HA	1.45	0.97
3:A:83:GLN:HB3	3:A:95:ASN:HD21	1.28	0.97
3:A:559:ILE:HG22	3:A:561:LYS:HG2	1.48	0.95
3:A:328:LYS:HG3	3:A:332:CYS:HB3	1.50	0.94
3:A:1413:TRP:HA	3:A:1416:VAL:HG12	1.50	0.94
3:A:340:TRP:O	3:A:344:GLU:HB3	1.68	0.93
3:A:1154:ILE:HG21	3:A:1164:LYS:HG3	1.51	0.93
3:A:691:LYS:HB3	3:A:694:THR:HA	1.50	0.92
3:A:1307:GLU:HA	3:A:1310:LEU:HB2	1.54	0.90
3:A:333:VAL:HA	3:A:337:LYS:HB2	1.52	0.89
3:A:1302:ASN:HA	3:A:1305:HIS:HB2	1.54	0.89
3:A:19:SER:HA	3:A:216:ASN:HB3	1.55	0.88
3:A:133:ARG:HH12	3:A:137:GLU:HB3	1.38	0.87
3:A:278:ARG:O	3:A:282:GLU:HB2	1.73	0.87
3:A:499:LEU:HD13	3:A:701:TYR:HE1	1.37	0.86
3:A:191:ARG:NH2	3:A:205:GLN:O	2.08	0.85
3:A:186:MET:SD	3:A:189:LYS:NZ	2.49	0.85
3:A:1356:ASN:HB3	3:A:1449:GLN:HE21	1.42	0.85
3:A:338:THR:HA	3:A:342:ASN:HB2	1.59	0.84
3:A:610:LYS:HA	3:A:684:LEU:HD21	1.60	0.84
3:A:1257:HIS:ND1	3:A:1364:ASN:O	2.09	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1301:LYS:HD3	3:A:1422:LYS:HD2	1.60	0.83
3:A:365:ARG:HH12	3:A:374:PHE:HB2	1.43	0.83
3:A:1199:GLU:HB3	3:A:1203:LYS:HG3	1.60	0.83
3:A:717:LYS:HA	3:A:750:ILE:HD11	1.59	0.82
3:A:294:LEU:HA	3:A:298:MET:HB2	1.61	0.82
3:A:854:LYS:HA	3:A:869:ALA:HB3	1.60	0.82
3:A:725:HIS:HA	3:A:730:ASN:HD21	1.43	0.81
3:A:1352:ILE:HD11	3:A:1442:PRO:HG2	1.62	0.81
3:A:562:LYS:HB2	3:A:575:ALA:HB1	1.60	0.81
3:A:276:PHE:O	3:A:280:LEU:N	2.13	0.81
3:A:235:LEU:HA	3:A:258:LYS:HG2	1.60	0.81
3:A:1278:TRP:HB2	3:A:1372:LEU:HD11	1.63	0.81
3:A:345:ASN:HB3	3:A:352:GLU:H	1.47	0.80
3:A:795:CYS:HB3	3:A:967:LYS:HD2	1.64	0.80
3:A:942:ASP:HA	3:A:946:VAL:HA	1.61	0.80
3:A:96:ILE:HD11	3:A:346:LYS:HB3	1.63	0.80
3:A:1125:GLN:HG3	3:A:1128:ASP:HB3	1.64	0.80
1:B:153:LEU:HB3	2:C:137:PHE:HD1	1.47	0.79
3:A:1193:GLU:O	3:A:1197:ASN:N	2.15	0.79
1:B:117:ARG:NH1	1:B:131:ASN:OD1	2.14	0.79
3:A:281:THR:HG23	3:A:285:GLU:HB3	1.64	0.79
3:A:1013:LYS:HB2	3:A:1018:ARG:HH22	1.47	0.79
3:A:989:SER:O	3:A:1110:GLN:NE2	2.16	0.79
3:A:1396:SER:HA	3:A:1399:GLU:HG2	1.63	0.78
3:A:1497:ILE:HG22	3:A:1499:GLY:H	1.47	0.78
3:A:1376:ILE:HD13	3:A:1380:ILE:HG13	1.66	0.78
3:A:1375:ASP:O	3:A:1379:ILE:N	2.16	0.78
3:A:1125:GLN:HA	3:A:1128:ASP:H	1.49	0.78
3:A:997:TYR:H	3:A:1003:GLU:HG3	1.48	0.77
3:A:234:ASP:O	3:A:238:LYS:NZ	2.17	0.77
3:A:925:THR:H	3:A:946:VAL:HG12	1.49	0.77
3:A:251:LYS:HB3	3:A:566:ASN:CB	2.08	0.77
3:A:524:GLN:HG3	3:A:527:CYS:HB2	1.67	0.76
3:A:563:SER:O	3:A:564:SER:C	2.28	0.76
3:A:872:THR:OG1	3:A:874:GLU:O	2.02	0.76
3:A:530:LYS:HD2	3:A:531:LEU:HB2	1.67	0.76
3:A:164:ASP:OD1	3:A:167:ARG:NH1	2.19	0.75
3:A:188:ALA:HA	3:A:191:ARG:HG2	1.68	0.75
3:A:1424:ASN:ND2	3:A:1430:SER:O	2.15	0.75
3:A:1471:ASN:HB3	3:A:1504:LYS:HD2	1.68	0.75
3:A:33:SER:HA	3:A:48:LYS:HZ2	1.50	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1126:ILE:O	3:A:1130:ASN:ND2	2.19	0.75
3:A:927:GLU:HB2	3:A:943:THR:HA	1.69	0.75
3:A:1933:CYS:H	3:A:1934:GLU:HG3	1.51	0.75
3:A:987:CYS:SG	3:A:995:ARG:N	2.57	0.75
3:A:1356:ASN:O	3:A:1360:GLY:N	2.20	0.75
3:A:499:LEU:HD13	3:A:701:TYR:CE1	2.20	0.74
3:A:1826:ARG:HG3	3:A:1831:GLY:HA2	1.67	0.74
3:A:1422:LYS:HA	3:A:1425:LYS:HG2	1.68	0.74
3:A:102:ARG:HH22	3:A:282:GLU:HG3	1.53	0.74
3:A:1627:ARG:NH2	3:A:1801:GLU:OE2	2.15	0.73
3:A:121:ASN:HA	3:A:124:PHE:HB3	1.69	0.73
1:B:220:THR:OG1	1:B:221:GLN:OE1	2.07	0.73
3:A:38:TYR:O	3:A:39:ARG:NH1	2.19	0.73
3:A:188:ALA:O	3:A:192:GLU:N	2.22	0.73
3:A:1355:LYS:HE3	3:A:1406:LYS:HE3	1.71	0.73
3:A:113:LEU:H	3:A:182:ASN:HD21	1.35	0.72
3:A:25:ASP:HA	3:A:28:LEU:HB3	1.70	0.72
1:B:49:ASP:OD2	1:B:93:ASN:ND2	2.22	0.72
3:A:802:LYS:O	3:A:805:ASP:N	2.17	0.72
3:A:1408:ILE:O	3:A:1412:MET:N	2.23	0.72
3:A:275:GLN:HG3	3:A:279:TRP:CZ3	2.25	0.72
3:A:830:PRO:HG3	3:A:928:LYS:HD3	1.70	0.72
3:A:32:PRO:O	3:A:48:LYS:NZ	2.23	0.71
3:A:939:GLN:H	3:A:943:THR:HG21	1.53	0.71
3:A:1268:ARG:NH2	3:A:1353:ASP:OD2	2.16	0.71
3:A:1380:ILE:O	3:A:1384:THR:OG1	2.08	0.71
3:A:195:LYS:HD3	3:A:201:TYR:HE1	1.54	0.71
3:A:277:LEU:HA	3:A:280:LEU:HB2	1.72	0.71
3:A:1356:ASN:HA	3:A:1359:LEU:HG	1.71	0.71
3:A:324:ASP:OD1	3:A:325:LYS:N	2.24	0.71
3:A:33:SER:HA	3:A:48:LYS:NZ	2.06	0.71
3:A:1042:ILE:HD11	3:A:1107:ILE:HD12	1.71	0.71
3:A:80:TRP:HA	3:A:97:CYS:HA	1.71	0.70
3:A:698:ASP:H	3:A:699:THR:HB	1.54	0.70
3:A:1893:ASN:ND2	3:A:1933:CYS:O	2.22	0.70
3:A:73:PRO:O	3:A:104:ARG:NH1	2.24	0.70
3:A:344:GLU:HA	3:A:347:TYR:HB2	1.73	0.70
3:A:972:GLU:HA	3:A:1102:LEU:HD21	1.74	0.70
3:A:1315:HIS:HD2	3:A:1342:GLY:HA3	1.56	0.70
3:A:1136:LYS:HE2	3:A:1140:SER:H	1.57	0.70
2:C:49:ALA:O	2:C:85:GLN:NE2	2.24	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1485:LYS:HE2	3:A:1489:SER:HB2	1.74	0.69
3:A:1252:LYS:HG3	3:A:1521:LYS:HG3	1.75	0.69
2:C:149:ALA:HB3	2:C:200:LEU:H	1.58	0.68
3:A:1594:SER:O	3:A:1664:ARG:NH2	2.27	0.68
3:A:573:GLU:OE2	3:A:841:ARG:NH1	2.26	0.68
3:A:1310:LEU:O	3:A:1314:TYR:HB3	1.93	0.68
3:A:1359:LEU:O	3:A:1373:GLN:NE2	2.25	0.68
3:A:111:GLU:HA	3:A:179:LEU:HD13	1.74	0.68
3:A:529:LYS:NZ	3:A:531:LEU:O	2.27	0.68
3:A:576:ASN:O	3:A:837:GLN:NE2	2.27	0.68
3:A:206:LYS:HB3	3:A:209:LYS:HB3	1.76	0.68
3:A:273:VAL:HG13	3:A:277:LEU:HD23	1.74	0.68
3:A:987:CYS:HB2	3:A:1005:CYS:HA	1.73	0.68
3:A:637:ASN:ND2	3:A:640:ASN:O	2.22	0.68
3:A:251:LYS:CB	3:A:566:ASN:HB2	2.14	0.68
3:A:271:ASP:O	3:A:278:ARG:NH2	2.26	0.68
3:A:583:ARG:NH2	3:A:765:GLU:OE1	2.27	0.67
3:A:1136:LYS:HE2	3:A:1139:VAL:HA	1.76	0.67
3:A:1411:GLU:HA	3:A:1414:ASP:HB2	1.75	0.67
3:A:691:LYS:HB3	3:A:694:THR:CA	2.21	0.67
3:A:293:ASN:HA	3:A:296:ASP:HB2	1.76	0.67
3:A:1823:PRO:HB3	3:A:1828:ASP:HB2	1.76	0.67
3:A:1325:ASN:O	3:A:1467:ARG:NH2	2.27	0.67
3:A:236:LEU:HD13	3:A:259:CYS:HA	1.76	0.67
3:A:1933:CYS:HB2	3:A:1934:GLU:HA	1.75	0.67
1:B:174:TYR:HE2	1:B:178:PRO:HA	1.60	0.67
3:A:864:SER:HA	3:A:1790:ILE:HG21	1.75	0.66
3:A:1246:GLU:O	3:A:1248:GLN:NE2	2.28	0.66
3:A:701:TYR:HB3	3:A:706:GLU:OE1	1.95	0.66
1:B:184:ASN:HD22	1:B:188:LEU:HD13	1.60	0.66
3:A:504:GLU:HG3	3:A:521:ASN:HD21	1.60	0.66
1:B:173:ASP:HA	1:B:204:LEU:HB3	1.76	0.66
3:A:984:GLN:HB3	3:A:1007:TYR:CE2	2.30	0.66
3:A:1154:ILE:HG22	3:A:1161:ASP:HA	1.78	0.66
3:A:1125:GLN:HG2	3:A:1137:LYS:O	1.96	0.65
3:A:1988:LEU:HG	3:A:1989:ASP:H	1.60	0.65
3:A:1827:ALA:O	3:A:1830:CYS:N	2.27	0.65
3:A:689:ILE:HD12	3:A:701:TYR:HB2	1.79	0.65
3:A:1412:MET:HA	3:A:1415:ALA:HB3	1.77	0.65
3:A:1938:GLY:O	3:A:1940:LEU:N	2.29	0.65
3:A:1013:LYS:O	3:A:1018:ARG:NH1	2.21	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:181:LYS:HA	3:A:184:LYS:HE2	1.77	0.65
3:A:1127:TYR:O	3:A:1131:LYS:NZ	2.24	0.65
3:A:1594:SER:OG	3:A:1635:GLU:OE2	2.12	0.65
3:A:1692:ARG:NH2	3:A:1903:ASN:OD1	2.27	0.65
3:A:698:ASP:N	3:A:699:THR:HB	2.10	0.65
3:A:951:SER:O	3:A:953:LEU:N	2.26	0.65
3:A:990:ALA:C	3:A:991:ARG:HE	2.05	0.65
3:A:1411:GLU:O	3:A:1415:ALA:N	2.29	0.65
2:C:229:ASN:HB3	2:C:232:GLU:HG3	1.77	0.65
3:A:244:SER:O	3:A:257:ARG:NH2	2.30	0.65
3:A:529:LYS:HG3	3:A:530:LYS:H	1.60	0.65
3:A:1321:ILE:HG21	3:A:1460:GLN:HG2	1.77	0.65
3:A:1252:LYS:NZ	3:A:1261:ASN:O	2.30	0.64
3:A:842:TYR:OH	3:A:889:LEU:HD21	1.97	0.64
1:B:110:THR:HG23	1:B:139:ILE:HA	1.78	0.64
3:A:256:CYS:HA	3:A:257:ARG:HG2	1.80	0.64
3:A:562:LYS:O	3:A:564:SER:N	2.31	0.64
3:A:1305:HIS:HE1	3:A:1423:ILE:HA	1.62	0.64
3:A:333:VAL:O	3:A:338:THR:OG1	2.15	0.64
3:A:560:TRP:HA	3:A:579:GLY:HA2	1.80	0.64
3:A:1096:LYS:HD2	3:A:1201:LYS:HG2	1.79	0.64
1:B:221:GLN:NE2	1:B:223:TYR:OH	2.31	0.64
3:A:1251:CYS:SG	3:A:1252:LYS:N	2.71	0.63
3:A:342:ASN:O	3:A:346:LYS:NZ	2.24	0.63
3:A:1496:LYS:NZ	3:A:1497:ILE:O	2.29	0.63
3:A:325:LYS:HA	3:A:328:LYS:HB3	1.80	0.63
3:A:600:GLU:O	3:A:603:LYS:NZ	2.27	0.63
3:A:583:ARG:NH1	3:A:654:ASP:OD2	2.31	0.63
3:A:587:LEU:HD13	3:A:655:TYR:HE1	1.62	0.63
3:A:274:PRO:O	3:A:278:ARG:N	2.25	0.63
3:A:924:THR:OG1	3:A:945:VAL:HG22	1.99	0.63
3:A:1202:CYS:N	3:A:1204:GLU:HA	2.13	0.63
3:A:1295:LEU:O	3:A:1299:LYS:N	2.25	0.63
3:A:1409:GLU:HA	3:A:1412:MET:HB3	1.81	0.63
3:A:1058:ILE:HG23	3:A:1201:LYS:HB2	1.81	0.63
1:B:70:ILE:HD13	1:B:91:ARG:HG3	1.81	0.62
3:A:1166:LYS:HD3	3:A:1168:ILE:HG12	1.81	0.62
3:A:1260:THR:HA	3:A:1363:VAL:HG12	1.81	0.62
3:A:1307:GLU:O	3:A:1311:LEU:N	2.33	0.62
1:B:121:ASN:ND2	3:A:958:TYR:OH	2.22	0.62
3:A:1320:ALA:HB3	3:A:1323:SER:HB3	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1391:ILE:O	3:A:1400:ASN:ND2	2.32	0.62
3:A:80:TRP:O	3:A:81:LYS:HD2	2.00	0.62
3:A:149:SER:HA	3:A:238:LYS:HD3	1.81	0.62
3:A:799:CYS:HB2	3:A:802:LYS:HA	1.82	0.62
3:A:850:LYS:HZ1	3:A:890:ILE:HD13	1.64	0.62
3:A:1280:LYS:O	3:A:1285:ARG:NH1	2.32	0.62
3:A:1418:CYS:HA	3:A:1421:THR:HG22	1.81	0.62
3:A:583:ARG:NH2	3:A:650:TYR:HB3	2.14	0.62
3:A:1484:LYS:HE2	3:A:1573:ILE:HG13	1.82	0.62
3:A:587:LEU:HD12	3:A:590:GLY:H	1.64	0.62
3:A:857:THR:OG1	3:A:871:SER:O	2.18	0.62
3:A:83:GLN:N	3:A:95:ASN:OD1	2.32	0.62
3:A:332:CYS:SG	3:A:336:TRP:N	2.73	0.62
3:A:562:LYS:C	3:A:564:SER:N	2.56	0.62
2:C:141:ASP:OD2	2:C:142:GLU:N	2.32	0.62
3:A:65:ASP:OD1	3:A:66:PRO:HD2	2.00	0.62
3:A:236:LEU:HB2	3:A:259:CYS:N	2.14	0.61
3:A:852:ASN:ND2	3:A:854:LYS:O	2.33	0.61
3:A:1304:ILE:HA	3:A:1307:GLU:HB3	1.81	0.61
1:B:229:HIS:CD2	1:B:231:PRO:HD2	2.36	0.61
3:A:1843:ALA:O	3:A:1847:ASN:ND2	2.33	0.61
3:A:132:ALA:HB1	3:A:226:ILE:HB	1.83	0.61
3:A:1550:ASN:HD22	3:A:1711:GLU:HG2	1.65	0.61
3:A:1863:TYR:HA	3:A:1866:ILE:HG22	1.81	0.61
3:A:1274:VAL:HG12	3:A:1278:TRP:H	1.65	0.61
3:A:1187:GLY:O	3:A:1190:ILE:HG22	2.00	0.61
3:A:200:LYS:NZ	3:A:209:LYS:O	2.33	0.61
3:A:1314:TYR:HA	3:A:1319:THR:OG1	2.01	0.61
3:A:1469:GLU:OE2	3:A:1473:ARG:NE	2.25	0.61
3:A:1581:TYR:N	3:A:1656:GLU:OE1	2.27	0.61
3:A:568:GLU:HG3	3:A:667:ASN:HB3	1.83	0.61
3:A:1296:LEU:O	3:A:1300:ILE:N	2.34	0.61
3:A:1301:LYS:HG2	3:A:1419:ALA:HA	1.82	0.61
2:C:164:LYS:NZ	2:C:166:GLN:OE1	2.34	0.61
3:A:278:ARG:HA	3:A:281:THR:HB	1.83	0.61
3:A:867:ASN:C	3:A:867:ASN:HD22	2.06	0.61
1:B:184:ASN:HD21	1:B:223:TYR:HD1	1.47	0.61
3:A:38:TYR:HE1	3:A:118:ILE:HB	1.65	0.61
3:A:182:ASN:OD1	3:A:185:GLN:NE2	2.34	0.61
3:A:983:ASN:HA	3:A:991:ARG:HB3	1.83	0.61
3:A:555:LYS:HD2	3:A:585:GLN:HG3	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1402:ASN:HB3	3:A:1406:LYS:HD3	1.83	0.60
2:C:54:TRP:CZ3	2:C:107:CYS:HB3	2.36	0.60
3:A:861:GLY:N	3:A:891:ASP:OD1	2.33	0.60
3:A:1237:GLY:H	3:A:1246:GLU:HA	1.67	0.60
3:A:925:THR:N	3:A:946:VAL:H	1.98	0.60
3:A:176:ASN:O	3:A:180:GLU:N	2.27	0.60
3:A:176:ASN:HA	3:A:179:LEU:HB3	1.82	0.60
3:A:873:ASP:OD1	3:A:874:GLU:N	2.33	0.60
3:A:1212:ILE:O	3:A:1417:ARG:NH1	2.34	0.60
3:A:13:GLU:HA	3:A:17:ALA:HB2	1.83	0.60
3:A:81:LYS:N	3:A:96:ILE:O	2.25	0.60
3:A:287:PHE:CD1	3:A:291:LYS:HE2	2.37	0.60
3:A:850:LYS:CE	3:A:890:ILE:HG21	2.32	0.60
3:A:1053:ALA:O	3:A:1059:ASP:HB2	2.00	0.60
3:A:1272:LEU:HB2	3:A:1354:TYR:HE1	1.67	0.60
3:A:277:LEU:HD12	3:A:280:LEU:HB2	1.84	0.60
3:A:1125:GLN:HB3	3:A:1129:ALA:CB	2.31	0.60
3:A:1564:TYR:CD2	3:A:1594:SER:HA	2.36	0.60
3:A:288:TYR:O	3:A:292:GLN:HB2	2.01	0.59
2:C:113:ALA:HB3	2:C:114:PRO:HD3	1.83	0.59
3:A:155:LEU:HD11	3:A:226:ILE:HG12	1.85	0.59
3:A:182:ASN:HA	3:A:185:GLN:HG3	1.84	0.59
3:A:689:ILE:HD13	3:A:707:LEU:HB2	1.84	0.59
3:A:686:GLY:O	3:A:687:LYS:C	2.45	0.59
3:A:1348:GLN:NE2	3:A:1437:CYS:SG	2.62	0.59
3:A:30:ALA:HB3	3:A:125:LEU:HD22	1.84	0.59
3:A:231:ARG:N	3:A:234:ASP:OD2	2.32	0.59
3:A:557:LYS:O	3:A:558:TRP:C	2.45	0.59
3:A:236:LEU:HB2	3:A:259:CYS:H	1.67	0.59
3:A:805:ASP:OD1	3:A:806:GLU:N	2.35	0.59
3:A:45:ASP:OD2	3:A:1901:ASN:ND2	2.35	0.59
3:A:1053:ALA:C	3:A:1055:ILE:H	2.11	0.59
3:A:1454:PHE:CE1	3:A:1522:GLN:HB3	2.38	0.59
3:A:1497:ILE:HG21	3:A:1501:CYS:HB3	1.85	0.59
3:A:1590:LYS:O	3:A:1664:ARG:NH1	2.35	0.59
3:A:787:SER:N	3:A:790:GLU:O	2.36	0.59
3:A:1274:VAL:HG11	3:A:1278:TRP:HB3	1.85	0.59
3:A:1316:ASP:C	3:A:1330:GLN:HG3	2.28	0.59
3:A:88:ASP:HB2	3:A:93:PRO:HA	1.83	0.59
3:A:185:GLN:HE22	3:A:186:MET:HE2	1.68	0.59
3:A:1361:THR:OG1	3:A:1449:GLN:OE1	2.11	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1655:LEU:HD13	3:A:1756:ILE:HD12	1.84	0.59
2:C:38:VAL:HG11	2:C:123:LEU:HD21	1.83	0.59
3:A:125:LEU:HG	3:A:129:LEU:HD13	1.83	0.59
3:A:275:GLN:OE1	3:A:278:ARG:NH1	2.35	0.59
3:A:509:ASN:HD22	3:A:513:SER:HB3	1.68	0.59
3:A:850:LYS:NZ	3:A:890:ILE:HD13	2.17	0.59
3:A:1147:PHE:CE2	3:A:1969:VAL:HG22	2.38	0.59
3:A:99:PRO:HD2	3:A:282:GLU:OE2	2.03	0.58
3:A:191:ARG:NH1	3:A:207:TYR:HA	2.18	0.58
3:A:1278:TRP:CD1	3:A:1371:LYS:HZ1	2.21	0.58
3:A:1406:LYS:HA	3:A:1409:GLU:HB3	1.85	0.58
3:A:1412:MET:O	3:A:1416:VAL:N	2.34	0.58
2:C:204:ASP:HA	2:C:207:LYS:HB2	1.85	0.58
3:A:281:THR:O	3:A:285:GLU:N	2.37	0.58
3:A:562:LYS:C	3:A:564:SER:H	2.11	0.58
3:A:659:ILE:HD11	3:A:712:TRP:HE3	1.67	0.58
1:B:102:MET:HE1	1:B:138:VAL:HG11	1.84	0.58
2:C:40:ILE:HD12	2:C:92:LEU:HD23	1.85	0.58
3:A:1304:ILE:HG22	3:A:1308:THR:HG23	1.84	0.58
3:A:1:MET:SD	3:A:2:ASP:N	2.77	0.58
3:A:1199:GLU:C	3:A:1201:LYS:H	2.11	0.58
3:A:1316:ASP:HB2	3:A:1340:PRO:HG3	1.86	0.58
3:A:1889:ILE:HD13	3:A:1941:ASP:HA	1.84	0.58
1:B:67:VAL:HG13	1:B:83:VAL:HG21	1.84	0.58
3:A:690:LYS:O	3:A:692:ASN:N	2.34	0.58
3:A:7:ILE:HG22	3:A:387:TYR:CE2	2.38	0.58
3:A:924:THR:CA	3:A:946:VAL:O	2.24	0.58
3:A:254:GLU:O	3:A:258:LYS:N	2.37	0.58
3:A:985:TRP:H	3:A:991:ARG:HG3	1.69	0.58
3:A:339:GLU:HA	3:A:343:GLN:HB2	1.85	0.58
3:A:1901:ASN:OD1	3:A:1902:GLY:N	2.37	0.58
3:A:725:HIS:HA	3:A:730:ASN:ND2	2.17	0.57
3:A:1096:LYS:HA	3:A:1100:TYR:HB3	1.85	0.57
3:A:1202:CYS:N	3:A:1204:GLU:OE1	2.38	0.57
3:A:1883:ILE:O	3:A:1883:ILE:HG13	2.05	0.57
1:B:217:SER:HB2	1:B:221:GLN:HE22	1.69	0.57
3:A:336:TRP:HA	3:A:339:GLU:HB3	1.85	0.57
3:A:1929:LYS:HB3	3:A:1930:GLU:HG3	1.87	0.57
1:B:87:PHE:CZ	1:B:102:MET:HG2	2.39	0.57
3:A:1201:LYS:HD3	3:A:1204:GLU:HB3	1.86	0.57
3:A:1715:TYR:OH	3:A:1719:LYS:NZ	2.23	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:293:ASN:OD1	3:A:297:ASP:HB2	2.03	0.57
3:A:1818:LYS:HA	3:A:1957:HIS:HE1	1.69	0.57
3:A:88:ASP:C	3:A:93:PRO:HB3	2.29	0.57
3:A:689:ILE:CD1	3:A:707:LEU:HB2	2.34	0.57
3:A:1282:TYR:HB3	3:A:1285:ARG:HB2	1.85	0.57
1:B:94:PRO:HB2	3:A:1055:ILE:HG12	1.86	0.57
3:A:341:GLU:O	3:A:345:ASN:ND2	2.38	0.57
3:A:659:ILE:HD11	3:A:712:TRP:CE3	2.40	0.57
3:A:863:SER:HB3	3:A:1879:ASP:OD1	2.05	0.57
3:A:102:ARG:HH12	3:A:282:GLU:CD	2.13	0.57
3:A:118:ILE:HD11	3:A:124:PHE:HB2	1.86	0.57
3:A:562:LYS:HB2	3:A:575:ALA:CB	2.34	0.57
3:A:575:ALA:O	3:A:577:THR:OG1	2.19	0.57
3:A:1235:TYR:HD1	3:A:1271:ASN:HD21	1.53	0.57
3:A:1984:LYS:C	3:A:1986:TYR:H	2.14	0.56
3:A:11:ILE:HA	3:A:14:TYR:HD2	1.70	0.56
3:A:178:ASN:O	3:A:182:ASN:HB2	2.06	0.56
3:A:689:ILE:HD11	3:A:703:SER:O	2.06	0.56
3:A:9:ASN:H	3:A:387:TYR:HE1	1.53	0.56
3:A:10:LYS:H	3:A:387:TYR:HE1	1.54	0.56
3:A:990:ALA:HA	3:A:1107:ILE:HD11	1.86	0.56
1:B:128:ALA:HB1	2:C:65:LEU:HD11	1.87	0.56
3:A:511:ARG:O	3:A:512:GLY:C	2.49	0.56
3:A:757:PRO:HB3	3:A:882:ILE:HD12	1.88	0.56
3:A:1120:LYS:O	3:A:1124:LYS:HG2	2.04	0.56
3:A:1236:ASP:O	3:A:1243:LYS:NZ	2.31	0.56
3:A:1320:ALA:O	3:A:1323:SER:OG	2.22	0.56
3:A:1386:GLN:HE21	3:A:1390:LYS:HA	1.71	0.56
3:A:184:LYS:HG3	3:A:207:TYR:CZ	2.40	0.56
3:A:591:ASN:HA	3:A:669:TYR:HD2	1.70	0.56
3:A:862:THR:HG22	3:A:1871:ASN:ND2	2.21	0.56
3:A:1339:LEU:HD22	3:A:1343:PHE:HD2	1.71	0.56
3:A:384:LEU:HB2	3:A:388:ILE:HG13	1.86	0.56
3:A:858:LYS:HD3	3:A:860:CYS:SG	2.46	0.56
3:A:1405:TRP:O	3:A:1409:GLU:HB2	2.06	0.56
3:A:862:THR:HG22	3:A:1871:ASN:HD21	1.71	0.56
3:A:1143:ASN:HB3	3:A:1973:LEU:HD21	1.88	0.55
3:A:1543:TYR:HB2	3:A:1546:CYS:SG	2.46	0.55
3:A:688:TYR:O	3:A:689:ILE:C	2.50	0.55
3:A:949:VAL:HG11	3:A:1867:TYR:OH	2.06	0.55
3:A:1118:TYR:OH	3:A:1139:VAL:O	2.16	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1339:LEU:HD22	3:A:1343:PHE:CD2	2.40	0.55
3:A:1402:ASN:HA	3:A:1405:TRP:HB3	1.88	0.55
3:A:1402:ASN:O	3:A:1406:LYS:HB2	2.05	0.55
3:A:1436:GLU:HG2	3:A:1437:CYS:H	1.69	0.55
3:A:85:ASN:HD21	3:A:94:GLU:HB2	1.70	0.55
3:A:1125:GLN:HA	3:A:1128:ASP:N	2.20	0.55
3:A:1345:HIS:HB3	3:A:1349:ARG:HG3	1.88	0.55
3:A:577:THR:CG2	3:A:841:ARG:HB2	2.36	0.55
2:C:166:GLN:HE21	2:C:167:TRP:H	1.54	0.55
3:A:80:TRP:O	3:A:94:GLU:HG2	2.06	0.55
3:A:328:LYS:O	3:A:332:CYS:N	2.36	0.55
1:B:71:ASN:O	1:B:91:ARG:NH1	2.40	0.55
3:A:82:CYS:H	3:A:95:ASN:H	1.55	0.55
3:A:113:LEU:H	3:A:182:ASN:ND2	2.03	0.55
3:A:231:ARG:HG2	3:A:234:ASP:CG	2.32	0.55
3:A:279:TRP:CD1	3:A:282:GLU:HB3	2.41	0.55
3:A:286:ASP:O	3:A:290:GLU:HG3	2.07	0.55
3:A:1308:THR:HA	3:A:1311:LEU:CB	2.36	0.55
3:A:127:ASP:OD1	3:A:128:VAL:N	2.40	0.55
3:A:180:GLU:HG2	3:A:184:LYS:HZ3	1.72	0.55
3:A:1768:VAL:HG21	3:A:1783:MET:HE2	1.88	0.55
3:A:187:PHE:HA	3:A:190:ILE:HG12	1.89	0.55
3:A:1299:LYS:HA	3:A:1303:ALA:H	1.72	0.55
3:A:1333:LYS:HE2	3:A:1341:LYS:HE2	1.88	0.55
3:A:113:LEU:HB2	3:A:186:MET:HG3	1.89	0.54
3:A:1315:HIS:CD2	3:A:1342:GLY:HA3	2.41	0.54
3:A:1599:LYS:HB2	3:A:1672:GLN:HB2	1.89	0.54
3:A:279:TRP:HB3	3:A:283:TRP:NE1	2.22	0.54
3:A:275:GLN:O	3:A:279:TRP:N	2.41	0.54
3:A:841:ARG:HE	3:A:845:HIS:CD2	2.26	0.54
3:A:55:THR:H	3:A:58:HIS:CD2	2.26	0.54
3:A:1310:LEU:O	3:A:1314:TYR:CB	2.55	0.54
3:A:1396:SER:O	3:A:1400:ASN:ND2	2.40	0.54
3:A:1465:ARG:NH1	3:A:1569:ASP:OD2	2.40	0.54
3:A:1719:LYS:O	3:A:1723:ILE:HG12	2.07	0.54
3:A:28:LEU:O	3:A:121:ASN:ND2	2.41	0.54
3:A:1821:CYS:SG	3:A:1838:CYS:HB2	2.47	0.54
2:C:52:LEU:HD13	2:C:90:PHE:CG	2.43	0.54
3:A:259:CYS:SG	3:A:262:TYR:HB2	2.48	0.54
3:A:690:LYS:C	3:A:692:ASN:H	2.15	0.54
3:A:691:LYS:CB	3:A:694:THR:HA	2.32	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:862:THR:HG21	3:A:891:ASP:H	1.72	0.54
3:A:1443:THR:OG1	3:A:1446:ASP:OD2	2.23	0.54
2:C:186:ASP:OD2	2:C:188:LYS:HG2	2.08	0.54
3:A:80:TRP:O	3:A:94:GLU:HA	2.08	0.54
3:A:680:ASN:C	3:A:682:GLY:N	2.62	0.54
3:A:1298:GLU:O	3:A:1302:ASN:N	2.22	0.54
3:A:1307:GLU:C	3:A:1311:LEU:H	2.16	0.54
3:A:1409:GLU:HG3	3:A:1412:MET:HB3	1.90	0.54
3:A:287:PHE:HD1	3:A:291:LYS:HB2	1.72	0.54
3:A:1305:HIS:CE1	3:A:1423:ILE:HA	2.43	0.54
3:A:1305:HIS:HA	3:A:1308:THR:OG1	2.08	0.54
3:A:1372:LEU:O	3:A:1376:ILE:HG12	2.07	0.54
3:A:31:ASP:O	3:A:33:SER:N	2.41	0.54
3:A:121:ASN:CB	3:A:214:TRP:HE1	2.21	0.54
3:A:288:TYR:HB3	3:A:397:TYR:OH	2.07	0.54
3:A:295:ILE:HA	3:A:299:GLU:HB2	1.90	0.54
3:A:691:LYS:HZ1	3:A:700:SER:HB3	1.73	0.54
3:A:939:GLN:N	3:A:943:THR:HG21	2.23	0.54
3:A:112:ASN:HB3	3:A:114:LYS:NZ	2.22	0.53
3:A:926:THR:HG22	3:A:944:LEU:HD12	1.89	0.53
3:A:1364:ASN:HB3	3:A:1369:ILE:HG22	1.91	0.53
3:A:1445:ASN:O	3:A:1530:TYR:OH	2.25	0.53
3:A:1483:GLU:OE2	3:A:1578:GLN:N	2.41	0.53
1:B:71:ASN:HB2	1:B:76:ASP:HB3	1.90	0.53
2:C:127:ARG:NE	2:C:128:THR:O	2.38	0.53
3:A:113:LEU:N	3:A:182:ASN:HD21	2.06	0.53
3:A:1396:SER:HB3	3:A:1400:ASN:ND2	2.22	0.53
3:A:1413:TRP:CH2	3:A:1442:PRO:HD3	2.43	0.53
3:A:1936:GLU:HB2	3:A:1939:PRO:HA	1.91	0.53
3:A:256:CYS:SG	3:A:257:ARG:NH1	2.81	0.53
3:A:337:LYS:HB3	3:A:341:GLU:OE2	2.08	0.53
3:A:345:ASN:HA	3:A:350:LEU:HA	1.91	0.53
3:A:559:ILE:C	3:A:561:LYS:H	2.16	0.53
3:A:927:GLU:OE2	3:A:933:ARG:N	2.33	0.53
2:C:27:PRO:HG2	2:C:30:LEU:HB2	1.89	0.53
3:A:191:ARG:NH1	3:A:210:LEU:HB3	2.24	0.53
3:A:281:THR:O	3:A:286:ASP:N	2.33	0.53
3:A:984:GLN:H	3:A:991:ARG:HB3	1.73	0.53
3:A:1240:PHE:CD1	3:A:1241:PRO:HA	2.43	0.53
2:C:111:ASN:ND2	2:C:112:ASN:OD1	2.42	0.53
3:A:1049:TYR:C	3:A:1053:ALA:HA	2.34	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1219:CYS:HB3	3:A:1422:LYS:HE2	1.91	0.53
3:A:1417:ARG:HA	3:A:1420:ILE:HG22	1.90	0.53
3:A:1822:ASP:CG	3:A:1823:PRO:HD3	2.33	0.53
1:B:153:LEU:HB3	2:C:137:PHE:CD1	2.36	0.53
3:A:59:SER:OG	3:A:60:ASP:N	2.41	0.53
3:A:129:LEU:HD23	3:A:225:VAL:HG21	1.90	0.53
3:A:262:TYR:CE2	3:A:573:GLU:HB2	2.42	0.53
3:A:1006:LYS:NZ	3:A:1011:ASP:HA	2.23	0.53
3:A:1385:PRO:HB3	3:A:1404:TRP:CE3	2.44	0.53
3:A:1615:ASN:ND2	3:A:1875:GLU:OE2	2.42	0.53
3:A:1984:LYS:HE3	3:A:1984:LYS:HA	1.89	0.53
3:A:1:MET:SD	3:A:3:SER:N	2.82	0.53
3:A:36:GLU:HG2	3:A:1781:LEU:HB3	1.91	0.53
2:C:168:LYS:HB3	2:C:171:ASN:HA	1.90	0.53
3:A:239:ARG:HH12	3:A:249:ARG:HH12	1.57	0.53
3:A:513:SER:O	3:A:514:SER:C	2.52	0.53
3:A:993:MET:HG2	3:A:1008:ASN:HD21	1.73	0.53
3:A:1202:CYS:H	3:A:1204:GLU:CD	2.16	0.53
3:A:1368:HIS:ND1	3:A:1371:LYS:HB3	2.24	0.53
3:A:38:TYR:HA	3:A:117:LYS:HE3	1.90	0.53
3:A:215:TRP:HZ3	3:A:272:TYR:HE1	1.57	0.53
3:A:689:ILE:HD11	3:A:703:SER:C	2.34	0.53
3:A:940:SER:O	3:A:943:THR:HG22	2.09	0.53
3:A:1121:PHE:O	3:A:1125:GLN:OE1	2.26	0.53
3:A:964:CYS:O	3:A:965:GLN:HG3	2.08	0.53
3:A:1369:ILE:HD12	3:A:1372:LEU:HD12	1.90	0.53
3:A:235:LEU:HD21	3:A:675:LEU:HD13	1.90	0.52
3:A:1015:THR:O	3:A:1018:ARG:NH1	2.41	0.52
3:A:1596:CYS:SG	3:A:1664:ARG:HG2	2.48	0.52
3:A:289:ARG:O	3:A:293:ASN:HB2	2.09	0.52
3:A:524:GLN:O	3:A:526:GLU:N	2.42	0.52
3:A:528:GLN:NE2	3:A:718:TYR:OH	2.42	0.52
3:A:587:LEU:HD13	3:A:655:TYR:CE1	2.44	0.52
3:A:1202:CYS:H	3:A:1204:GLU:HA	1.72	0.52
3:A:279:TRP:HB3	3:A:283:TRP:CD1	2.45	0.52
3:A:499:LEU:HD11	3:A:522:LYS:HB3	1.91	0.52
3:A:1215:SER:HB3	3:A:1216:GLU:HG3	1.91	0.52
2:C:109:LYS:NZ	2:C:114:PRO:HD2	2.25	0.52
3:A:164:ASP:OD2	3:A:278:ARG:NH1	2.41	0.52
3:A:270:LEU:O	3:A:273:VAL:HB	2.09	0.52
3:A:632:TYR:O	3:A:637:ASN:N	2.41	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1092:ASN:HA	3:A:1097:CYS:HB3	1.90	0.52
3:A:1269:THR:O	3:A:1272:LEU:HD22	2.09	0.52
3:A:1752:ASP:OD1	3:A:1753:ARG:N	2.37	0.52
3:A:180:GLU:HG2	3:A:184:LYS:NZ	2.24	0.52
3:A:1298:GLU:HA	3:A:1301:LYS:HD2	1.90	0.52
3:A:1408:ILE:C	3:A:1412:MET:H	2.16	0.52
3:A:121:ASN:O	3:A:125:LEU:N	2.43	0.52
3:A:687:LYS:O	3:A:688:TYR:C	2.53	0.52
3:A:850:LYS:HD2	3:A:864:SER:HB2	1.92	0.52
3:A:1129:ALA:O	3:A:1133:SER:N	2.43	0.52
3:A:1314:TYR:CD2	3:A:1320:ALA:HB2	2.45	0.52
3:A:1474:GLU:HA	3:A:1478:ILE:HB	1.90	0.52
3:A:1741:TRP:HA	3:A:1746:THR:HG21	1.91	0.52
3:A:29:LYS:HB3	3:A:217:ALA:HB1	1.91	0.52
3:A:79:GLN:OE1	3:A:81:LYS:NZ	2.43	0.52
3:A:1345:HIS:NE2	3:A:1543:TYR:HE1	2.07	0.52
3:A:1636:LEU:O	3:A:1640:ILE:HG12	2.10	0.52
3:A:159:PHE:HE1	3:A:222:VAL:HG13	1.74	0.52
3:A:207:TYR:HB3	3:A:211:ARG:NH1	2.25	0.52
3:A:852:ASN:OD1	3:A:853:ARG:N	2.41	0.52
3:A:1029:VAL:HG21	3:A:1959:MET:HE1	1.92	0.52
3:A:1277:LEU:O	3:A:1288:ILE:HG23	2.10	0.51
3:A:1420:ILE:HD12	3:A:1423:ILE:HB	1.92	0.51
3:A:1356:ASN:HD22	3:A:1359:LEU:HD11	1.74	0.51
3:A:82:CYS:HB2	3:A:96:ILE:HB	1.93	0.51
3:A:167:ARG:C	3:A:211:ARG:HE	2.19	0.51
3:A:1666:ALA:HB2	3:A:1764:MET:SD	2.49	0.51
3:A:935:LYS:HG3	3:A:936:SER:N	2.25	0.51
3:A:1627:ARG:NH1	3:A:1697:ASP:OD2	2.32	0.51
3:A:510:LYS:HE2	3:A:510:LYS:HA	1.91	0.51
3:A:559:ILE:HG22	3:A:561:LYS:CG	2.31	0.51
3:A:562:LYS:HZ3	3:A:576:ASN:HB2	1.76	0.51
3:A:1821:CYS:HA	3:A:1838:CYS:HB2	1.93	0.51
3:A:631:ARG:O	3:A:635:ASN:HB3	2.09	0.51
3:A:804:LYS:NZ	3:A:966:CYS:SG	2.82	0.51
1:B:119:LEU:HD12	1:B:120:ARG:HG3	1.91	0.51
3:A:203:LYS:HA	3:A:204:ASP:C	2.36	0.51
3:A:207:TYR:O	3:A:211:ARG:HG2	2.10	0.51
3:A:251:LYS:HE3	3:A:566:ASN:O	2.11	0.51
3:A:1125:GLN:CA	3:A:1129:ALA:H	2.24	0.51
3:A:1550:ASN:ND2	3:A:1711:GLU:O	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1814:PHE:CE2	3:A:1953:LYS:HE2	2.45	0.51
3:A:529:LYS:HB3	3:A:614:LEU:HD23	1.92	0.51
3:A:942:ASP:OD1	3:A:947:VAL:N	2.43	0.51
3:A:1313:GLU:O	3:A:1317:THR:OG1	2.12	0.51
3:A:1436:GLU:OE1	3:A:1436:GLU:N	2.38	0.51
2:C:21:ILE:HG21	2:C:46:GLN:HG2	1.93	0.51
3:A:95:ASN:CG	3:A:346:LYS:HE3	2.36	0.51
1:B:46:PHE:HE1	1:B:117:ARG:HE	1.58	0.50
1:B:48:PHE:HD2	1:B:96:SER:HA	1.75	0.50
3:A:537:SER:O	3:A:538:LEU:HG	2.11	0.50
3:A:680:ASN:C	3:A:682:GLY:H	2.19	0.50
3:A:682:GLY:O	3:A:683:LYS:C	2.54	0.50
3:A:988:GLY:HA2	3:A:1110:GLN:HG3	1.93	0.50
3:A:1262:GLY:HA2	3:A:1525:LYS:HE3	1.93	0.50
1:B:117:ARG:HD3	1:B:131:ASN:HB2	1.93	0.50
3:A:787:SER:OG	3:A:798:GLU:OE2	2.14	0.50
3:A:1199:GLU:HA	3:A:1202:CYS:O	2.11	0.50
3:A:1204:GLU:N	3:A:1205:ASN:HA	2.25	0.50
2:C:177:ASN:ND2	2:C:198:LEU:HD11	2.26	0.50
3:A:191:ARG:NE	3:A:205:GLN:HB3	2.26	0.50
3:A:277:LEU:HD22	3:A:373:PHE:CZ	2.46	0.50
3:A:562:LYS:NZ	3:A:576:ASN:HB2	2.26	0.50
3:A:1237:GLY:N	3:A:1246:GLU:HG3	2.26	0.50
3:A:1356:ASN:HB3	3:A:1449:GLN:NE2	2.21	0.50
3:A:1412:MET:O	3:A:1412:MET:HE3	2.11	0.50
3:A:925:THR:O	3:A:946:VAL:HG12	2.10	0.50
3:A:770:PHE:CZ	3:A:953:LEU:HD23	2.47	0.50
3:A:1305:HIS:CE1	3:A:1427:ASN:HB2	2.47	0.50
3:A:1839:LYS:HG3	3:A:1964:VAL:HG22	1.93	0.50
3:A:38:TYR:CE1	3:A:118:ILE:HB	2.44	0.50
3:A:80:TRP:CD1	3:A:94:GLU:HB3	2.46	0.50
3:A:291:LYS:HD2	3:A:339:GLU:OE2	2.12	0.50
3:A:694:THR:O	3:A:695:ALA:HB2	2.10	0.50
3:A:905:LEU:HD22	3:A:909:ILE:HD11	1.94	0.50
3:A:1056:SER:HB3	3:A:1057:CYS:HB2	1.93	0.50
3:A:1124:LYS:O	3:A:1127:TYR:HB3	2.12	0.50
3:A:1721:ASN:OD1	3:A:1738:ARG:NH1	2.44	0.50
3:A:1939:PRO:O	3:A:1941:ASP:N	2.45	0.50
3:A:1977:ASP:OD1	3:A:1978:ASN:N	2.44	0.50
1:B:31:VAL:HG21	1:B:105:LEU:HD12	1.93	0.50
2:C:23:MET:SD	2:C:109:LYS:HG2	2.52	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:504:GLU:HG3	3:A:521:ASN:ND2	2.27	0.50
3:A:894:LEU:HD11	3:A:903:ASN:HD22	1.75	0.50
3:A:1209:ASP:HB3	3:A:1210:THR:OG1	2.11	0.50
3:A:1285:ARG:HG2	3:A:1287:ASN:HA	1.94	0.50
1:B:119:LEU:HB3	1:B:130:GLY:HA3	1.93	0.50
3:A:51:ILE:HG12	3:A:221:LYS:HE3	1.94	0.50
3:A:219:ARG:HH21	3:A:266:VAL:HG21	1.76	0.50
3:A:1657:THR:HA	3:A:1660:ILE:HG22	1.94	0.50
3:A:235:LEU:HD12	3:A:258:LYS:HG2	1.94	0.49
3:A:290:GLU:OE2	3:A:291:LYS:NZ	2.45	0.49
3:A:968:ILE:HB	3:A:969:PRO:HD2	1.94	0.49
3:A:1142:SER:HB3	3:A:1187:GLY:H	1.77	0.49
3:A:1414:ASP:O	3:A:1417:ARG:HG2	2.12	0.49
3:A:1489:SER:HA	3:A:1498:GLN:HG2	1.94	0.49
3:A:1538:LEU:O	3:A:1542:ASN:ND2	2.44	0.49
3:A:290:GLU:OE2	3:A:291:LYS:HG3	2.12	0.49
3:A:1123:SER:C	3:A:1126:ILE:H	2.19	0.49
3:A:1215:SER:HB3	3:A:1216:GLU:CG	2.42	0.49
3:A:1359:LEU:HD12	3:A:1360:GLY:N	2.28	0.49
3:A:1376:ILE:HA	3:A:1380:ILE:HB	1.92	0.49
3:A:95:ASN:ND2	3:A:346:LYS:HE3	2.27	0.49
3:A:256:CYS:HA	3:A:257:ARG:CG	2.41	0.49
3:A:287:PHE:HD1	3:A:291:LYS:HE2	1.77	0.49
3:A:560:TRP:O	3:A:576:ASN:HA	2.11	0.49
3:A:562:LYS:CB	3:A:575:ALA:HB1	2.36	0.49
3:A:563:SER:O	3:A:565:GLY:N	2.45	0.49
3:A:697:GLN:N	3:A:699:THR:HB	2.27	0.49
3:A:1398:THR:O	3:A:1402:ASN:HB2	2.12	0.49
3:A:1308:THR:HB	3:A:1429:ASN:HD21	1.77	0.49
3:A:1310:LEU:HD22	3:A:1314:TYR:HB2	1.93	0.49
3:A:1325:ASN:HD21	3:A:1328:LYS:CG	2.25	0.49
3:A:558:TRP:HB2	3:A:825:GLY:O	2.13	0.49
2:C:206:GLU:HG3	2:C:230:ARG:NH1	2.28	0.49
3:A:637:ASN:HD21	3:A:640:ASN:C	2.18	0.49
3:A:788:CYS:O	3:A:789:LYS:NZ	2.42	0.49
3:A:1485:LYS:HB2	3:A:1489:SER:HB2	1.94	0.49
3:A:1933:CYS:SG	3:A:1936:GLU:HB3	2.51	0.49
3:A:674:GLU:OE2	3:A:708:ARG:NH1	2.27	0.49
3:A:1500:ALA:O	3:A:1503:ARG:NH1	2.45	0.49
1:B:25:GLU:HA	1:B:40:SER:O	2.13	0.49
1:B:181:VAL:HG22	1:B:227:VAL:HG12	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:216:ASN:O	3:A:219:ARG:HG2	2.13	0.49
3:A:691:LYS:O	3:A:692:ASN:C	2.55	0.49
3:A:699:THR:HG23	3:A:700:SER:O	2.13	0.49
3:A:1373:GLN:O	3:A:1377:LYS:HG2	2.12	0.49
3:A:1377:LYS:O	3:A:1381:GLU:HB2	2.13	0.49
3:A:1582:TYR:CD2	3:A:1589:LYS:HB2	2.47	0.49
3:A:817:CYS:SG	3:A:930:ASN:HB2	2.52	0.49
3:A:867:ASN:C	3:A:867:ASN:ND2	2.71	0.49
3:A:982:MET:H	3:A:991:ARG:NH1	2.11	0.49
3:A:1100:TYR:C	3:A:1102:LEU:H	2.20	0.49
2:C:31:SER:OG	2:C:124:GLU:OE2	2.28	0.48
3:A:76:ASP:HB2	3:A:104:ARG:HH22	1.77	0.48
3:A:289:ARG:O	3:A:293:ASN:CB	2.61	0.48
3:A:633:PRO:HA	3:A:634:GLN:HA	1.60	0.48
3:A:1626:PRO:O	3:A:1630:GLN:HG2	2.13	0.48
3:A:160:ALA:HB1	3:A:278:ARG:CZ	2.43	0.48
3:A:255:LEU:O	3:A:257:ARG:NH1	2.38	0.48
2:C:135:PHE:HB2	2:C:154:LEU:HB3	1.95	0.48
3:A:559:ILE:HD11	3:A:585:GLN:OE1	2.13	0.48
3:A:567:GLU:CD	3:A:567:GLU:H	2.21	0.48
3:A:1118:TYR:HA	3:A:1121:PHE:HB3	1.94	0.48
3:A:1406:LYS:HA	3:A:1409:GLU:CB	2.42	0.48
3:A:1959:MET:HA	3:A:1959:MET:HE2	1.96	0.48
2:C:206:GLU:HA	2:C:230:ARG:CZ	2.43	0.48
3:A:116:ASP:HB3	3:A:119:ARG:HH22	1.78	0.48
3:A:524:GLN:HB2	3:A:701:TYR:OH	2.13	0.48
3:A:989:SER:H	3:A:1110:GLN:CD	2.21	0.48
3:A:1133:SER:HB2	3:A:1134:GLN:HG2	1.95	0.48
3:A:1311:LEU:HD21	3:A:1339:LEU:HB2	1.95	0.48
3:A:1688:CYS:SG	3:A:1783:MET:HG2	2.54	0.48
2:C:108:GLN:HG3	2:C:117:PHE:CE1	2.49	0.48
3:A:524:GLN:OE1	3:A:701:TYR:CZ	2.67	0.48
3:A:559:ILE:CG2	3:A:561:LYS:HG2	2.30	0.48
3:A:1457:TRP:CH2	3:A:1519:TRP:HB2	2.49	0.48
3:A:767:VAL:HG11	3:A:901:LEU:HD21	1.94	0.48
3:A:1106:LYS:HB3	3:A:1110:GLN:NE2	2.28	0.48
1:B:58:GLN:HB2	1:B:64:LEU:HD23	1.95	0.48
3:A:80:TRP:C	3:A:81:LYS:HD2	2.38	0.48
3:A:125:LEU:HG	3:A:129:LEU:CD1	2.43	0.48
3:A:1005:CYS:HB2	3:A:1114:GLN:NE2	2.29	0.48
3:A:1497:ILE:HB	3:A:1502:LYS:HE2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:375:GLU:HA	3:A:380:ASN:HB3	1.95	0.48
3:A:1057:CYS:SG	3:A:1058:ILE:HB	2.53	0.48
3:A:1149:CYS:SG	3:A:1150:TRP:N	2.87	0.48
3:A:1408:ILE:HB	3:A:1411:GLU:HB3	1.94	0.48
3:A:60:ASP:O	3:A:64:TYR:HB3	2.13	0.48
3:A:1420:ILE:HG12	3:A:1436:GLU:HA	1.95	0.48
3:A:1477:THR:OG1	3:A:1645:GLU:OE1	2.28	0.48
2:C:55:TYR:HE1	2:C:108:GLN:HB3	1.79	0.48
2:C:163:ALA:HB2	2:C:217:HIS:HD2	1.79	0.48
3:A:591:ASN:HA	3:A:669:TYR:CD2	2.48	0.48
3:A:1726:SER:N	3:A:1729:THR:OG1	2.46	0.48
3:A:102:ARG:NH2	3:A:282:GLU:HG3	2.27	0.47
3:A:560:TRP:HH2	3:A:838:ILE:CG1	2.27	0.47
3:A:1308:THR:HA	3:A:1311:LEU:HB2	1.96	0.47
3:A:5:SER:HB3	3:A:384:LEU:HD21	1.96	0.47
3:A:168:GLY:HA3	3:A:211:ARG:HH21	1.78	0.47
3:A:580:LEU:O	3:A:585:GLN:NE2	2.46	0.47
3:A:691:LYS:HB3	3:A:694:THR:HG23	1.95	0.47
3:A:1164:LYS:HD3	3:A:1972:GLN:CD	2.39	0.47
3:A:1339:LEU:HD22	3:A:1343:PHE:HB3	1.95	0.47
1:B:228:ASN:HB3	1:B:230:LYS:NZ	2.29	0.47
3:A:1404:TRP:O	3:A:1408:ILE:HG12	2.14	0.47
3:A:1757:ARG:NH2	3:A:1788:ILE:O	2.47	0.47
3:A:166:ILE:O	3:A:211:ARG:HD2	2.14	0.47
3:A:277:LEU:HD22	3:A:373:PHE:CE1	2.49	0.47
3:A:1824:PRO:HG2	3:A:1832:ASP:H	1.79	0.47
3:A:275:GLN:O	3:A:275:GLN:NE2	2.44	0.47
3:A:1799:LEU:HD21	3:A:1888:VAL:HG23	1.95	0.47
1:B:224:ILE:HG22	1:B:239:LYS:HA	1.96	0.47
3:A:235:LEU:HD23	3:A:238:LYS:HE3	1.97	0.47
3:A:255:LEU:O	3:A:257:ARG:HD3	2.14	0.47
3:A:632:TYR:HB2	3:A:633:PRO:HD2	1.97	0.47
3:A:1250:ILE:HG12	3:A:1265:ILE:HB	1.95	0.47
3:A:1418:CYS:O	3:A:1422:LYS:HG2	2.14	0.47
3:A:1476:CYS:HA	3:A:1480:GLY:HA3	1.97	0.47
1:B:146:LYS:HD2	1:B:147:GLY:O	2.14	0.47
3:A:111:GLU:OE1	3:A:175:THR:OG1	2.33	0.47
3:A:187:PHE:HE2	3:A:191:ARG:HH11	1.62	0.47
3:A:1109:ASP:OD2	3:A:1113:LYS:NZ	2.47	0.47
3:A:1316:ASP:O	3:A:1330:GLN:HG3	2.14	0.47
3:A:1324:LYS:HB3	3:A:1467:ARG:NH2	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1454:PHE:HE1	3:A:1522:GLN:HB3	1.79	0.47
3:A:202:PRO:HB2	3:A:206:LYS:HG2	1.97	0.47
3:A:691:LYS:O	3:A:694:THR:N	2.48	0.47
3:A:1111:TRP:O	3:A:1115:LYS:N	2.29	0.47
3:A:1274:VAL:CG1	3:A:1278:TRP:H	2.28	0.47
3:A:1278:TRP:HA	3:A:1287:ASN:HB3	1.95	0.47
3:A:1633:LEU:HD11	3:A:1712:TYR:HB3	1.96	0.47
3:A:102:ARG:HA	3:A:105:LEU:CD1	2.45	0.47
3:A:254:GLU:HB3	3:A:258:LYS:O	2.15	0.47
3:A:365:ARG:NH2	3:A:370:VAL:O	2.48	0.47
3:A:562:LYS:HE2	3:A:576:ASN:ND2	2.30	0.47
3:A:617:CYS:HA	3:A:620:VAL:HG12	1.97	0.47
3:A:1499:GLY:HA2	3:A:1502:LYS:HB2	1.97	0.47
3:A:80:TRP:HB3	3:A:97:CYS:SG	2.55	0.47
3:A:164:ASP:O	3:A:168:GLY:N	2.48	0.47
3:A:236:LEU:HD22	3:A:260:GLY:N	2.30	0.47
3:A:690:LYS:C	3:A:692:ASN:N	2.73	0.47
3:A:1059:ASP:CG	3:A:1096:LYS:HD3	2.40	0.47
3:A:1550:ASN:ND2	3:A:1711:GLU:HG2	2.30	0.47
3:A:1754:LYS:NZ	3:A:1762:ASP:OD2	2.38	0.47
3:A:18:LYS:HB3	3:A:216:ASN:ND2	2.30	0.46
3:A:244:SER:OG	3:A:248:ASP:OD1	2.25	0.46
3:A:925:THR:O	3:A:946:VAL:HB	2.14	0.46
3:A:1397:SER:O	3:A:1401:VAL:HG22	2.15	0.46
2:C:151:VAL:HB	2:C:198:LEU:HB3	1.97	0.46
3:A:1114:GLN:NE2	3:A:1117:ASN:HD22	2.13	0.46
3:A:1305:HIS:CE1	3:A:1423:ILE:HG12	2.50	0.46
3:A:1312:TYR:O	3:A:1316:ASP:HB3	2.15	0.46
3:A:1419:ALA:O	3:A:1423:ILE:HG13	2.15	0.46
3:A:99:PRO:HB2	3:A:101:ARG:HB3	1.97	0.46
3:A:666:ASP:OD2	3:A:671:LYS:HE2	2.15	0.46
3:A:967:LYS:NZ	3:A:968:ILE:HG12	2.30	0.46
3:A:1348:GLN:O	3:A:1352:ILE:HB	2.16	0.46
3:A:1982:ASP:HA	3:A:1990:ARG:C	2.40	0.46
1:B:175:PHE:HB3	1:B:204:LEU:HD13	1.97	0.46
3:A:12:GLU:OE1	3:A:12:GLU:N	2.44	0.46
3:A:252:ASN:OD1	3:A:253:PHE:N	2.43	0.46
3:A:632:TYR:HA	3:A:636:LYS:HB2	1.97	0.46
3:A:689:ILE:HG13	3:A:702:SER:O	2.14	0.46
3:A:798:GLU:HG3	3:A:966:CYS:HB3	1.97	0.46
3:A:999:ASN:ND2	3:A:1001:ASN:O	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:143:GLN:O	2:C:146:SER:OG	2.15	0.46
3:A:365:ARG:HH12	3:A:374:PHE:CB	2.21	0.46
3:A:1092:ASN:HB3	3:A:1094:LYS:O	2.14	0.46
3:A:1133:SER:HA	3:A:1134:GLN:HA	1.68	0.46
3:A:1203:LYS:HB3	3:A:1205:ASN:OD1	2.16	0.46
1:B:93:ASN:ND2	3:A:1615:ASN:OD1	2.49	0.46
3:A:85:ASN:ND2	3:A:94:GLU:HB2	2.30	0.46
3:A:1096:LYS:HD2	3:A:1201:LYS:CG	2.45	0.46
3:A:1106:LYS:HE3	3:A:1110:GLN:HE22	1.80	0.46
3:A:1257:HIS:CD2	3:A:1265:ILE:HG13	2.51	0.46
1:B:145:THR:HA	1:B:176:PRO:HD3	1.97	0.46
1:B:212:THR:HG21	2:C:156:ASN:ND2	2.30	0.46
3:A:200:LYS:HE3	3:A:210:LEU:HD13	1.98	0.46
3:A:291:LYS:O	3:A:294:LEU:HB2	2.15	0.46
3:A:388:ILE:HG22	3:A:389:LYS:HG2	1.98	0.46
3:A:614:LEU:O	3:A:618:LEU:HD23	2.16	0.46
3:A:615:ALA:O	3:A:619:ILE:HG12	2.15	0.46
3:A:1794:GLN:HG3	3:A:1797:ARG:NH2	2.31	0.46
3:A:1954:TYR:OH	3:A:1961:CYS:SG	2.59	0.46
2:C:184:GLU:HA	2:C:184:GLU:OE2	2.16	0.46
3:A:83:GLN:HB3	3:A:95:ASN:ND2	2.12	0.46
3:A:170:ASP:HA	3:A:279:TRP:HH2	1.81	0.46
3:A:258:LYS:HE2	3:A:674:GLU:HG2	1.98	0.46
3:A:864:SER:HA	3:A:1790:ILE:CG2	2.44	0.46
3:A:978:ARG:HG3	3:A:980:GLU:OE2	2.16	0.46
3:A:1092:ASN:C	3:A:1094:LYS:H	2.23	0.46
3:A:24:ILE:HG22	3:A:24:ILE:O	2.16	0.46
3:A:148:SER:O	3:A:150:ASN:N	2.42	0.46
3:A:380:ASN:CG	3:A:381:TYR:H	2.23	0.46
3:A:653:ALA:HB2	3:A:753:ILE:HG23	1.98	0.46
3:A:767:VAL:HG21	3:A:901:LEU:HD21	1.98	0.46
3:A:1094:LYS:HD2	3:A:1096:LYS:HE2	1.98	0.46
3:A:1670:TRP:CH2	3:A:1780:PRO:HG3	2.49	0.46
3:A:1822:ASP:HB3	3:A:1957:HIS:CE1	2.50	0.46
2:C:158:PHE:HD2	2:C:217:HIS:HE2	1.64	0.46
3:A:1125:GLN:HA	3:A:1129:ALA:H	1.81	0.46
3:A:1424:ASN:HA	3:A:1430:SER:O	2.16	0.46
3:A:1824:PRO:HD2	3:A:1828:ASP:HA	1.98	0.46
3:A:273:VAL:HG13	3:A:277:LEU:CD2	2.45	0.45
3:A:690:LYS:HE3	3:A:690:LYS:HB3	1.37	0.45
3:A:696:GLU:C	3:A:699:THR:HB	2.41	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1667:TYR:OH	3:A:1671:LYS:NZ	2.42	0.45
3:A:319:CYS:HA	3:A:322:CYS:SG	2.57	0.45
3:A:779:LYS:O	3:A:783:THR:HG23	2.16	0.45
3:A:939:GLN:H	3:A:943:THR:CG2	2.25	0.45
3:A:1214:LYS:HG3	3:A:1414:ASP:OD2	2.16	0.45
3:A:38:TYR:CD2	3:A:59:SER:HA	2.52	0.45
3:A:185:GLN:NE2	3:A:186:MET:HG2	2.30	0.45
3:A:350:LEU:CB	3:A:355:LYS:H	2.30	0.45
3:A:894:LEU:HA	3:A:899:SER:OG	2.16	0.45
3:A:1136:LYS:HE2	3:A:1139:VAL:CA	2.46	0.45
3:A:1252:LYS:HG3	3:A:1521:LYS:HE2	1.97	0.45
2:C:40:ILE:O	2:C:91:THR:HA	2.16	0.45
3:A:367:ASP:HB3	3:A:371:LYS:HB2	1.98	0.45
3:A:562:LYS:O	3:A:563:SER:C	2.60	0.45
3:A:998:LYS:HD2	3:A:998:LYS:HA	1.78	0.45
3:A:1311:LEU:HG	3:A:1340:PRO:HG2	1.99	0.45
3:A:32:PRO:HB2	3:A:47:LEU:HD23	1.98	0.45
3:A:1814:PHE:CZ	3:A:1953:LYS:HB3	2.51	0.45
3:A:1965:TYR:O	3:A:1969:VAL:HG23	2.17	0.45
2:C:144:LEU:HD11	2:C:205:TYR:CE2	2.52	0.45
3:A:80:TRP:HD1	3:A:94:GLU:C	2.25	0.45
3:A:344:GLU:C	3:A:347:TYR:H	2.25	0.45
3:A:562:LYS:HE2	3:A:576:ASN:HD22	1.82	0.45
3:A:582:PRO:HA	3:A:585:GLN:HG2	1.99	0.45
3:A:859:ASN:N	3:A:891:ASP:OD2	2.46	0.45
3:A:971:ASN:HB3	3:A:1098:LYS:HG2	1.97	0.45
3:A:993:MET:HG3	3:A:994:LYS:N	2.30	0.45
3:A:1224:THR:OG1	3:A:1225:ASN:N	2.49	0.45
3:A:1325:ASN:HD21	3:A:1328:LYS:HG2	1.82	0.45
3:A:1409:GLU:HA	3:A:1412:MET:CB	2.46	0.45
1:B:166:ALA:HB3	2:C:137:PHE:HZ	1.82	0.45
3:A:111:GLU:HG2	3:A:179:LEU:HB2	1.98	0.45
3:A:987:CYS:HG	3:A:995:ARG:H	1.61	0.45
3:A:1103:TRP:HA	3:A:1106:LYS:HB2	1.97	0.45
3:A:1855:GLU:O	3:A:1859:MET:HG3	2.17	0.45
3:A:1960:LYS:HA	3:A:1963:GLU:HG2	1.98	0.45
3:A:1299:LYS:HB3	3:A:1303:ALA:HB2	1.98	0.45
3:A:1404:TRP:C	3:A:1408:ILE:HG12	2.42	0.45
1:B:200:GLN:HG2	1:B:204:LEU:O	2.17	0.45
2:C:208:HIS:O	2:C:230:ARG:NE	2.33	0.45
3:A:327:LYS:HA	3:A:327:LYS:HD2	1.76	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:690:LYS:O	3:A:690:LYS:HG2	2.16	0.45
3:A:935:LYS:HE2	3:A:938:SER:O	2.16	0.45
3:A:1206:GLU:HB2	3:A:1207:SER:C	2.42	0.45
3:A:247:SER:OG	3:A:391:ASP:OD1	2.30	0.45
3:A:293:ASN:O	3:A:297:ASP:N	2.48	0.45
3:A:345:ASN:HD22	3:A:352:GLU:HG3	1.82	0.44
3:A:679:ASN:O	3:A:683:LYS:HG2	2.17	0.44
3:A:984:GLN:H	3:A:991:ARG:CB	2.30	0.44
3:A:1007:TYR:HB3	3:A:1010:VAL:HG12	1.99	0.44
3:A:1834:SER:H	3:A:1837:GLU:CD	2.25	0.44
2:C:161:ARG:HH12	2:C:182:VAL:HG11	1.81	0.44
3:A:509:ASN:HD22	3:A:513:SER:CB	2.31	0.44
3:A:935:LYS:HG2	3:A:938:SER:C	2.42	0.44
3:A:1455:LYS:HB3	3:A:1543:TYR:OH	2.17	0.44
3:A:710:SER:O	3:A:714:THR:HG22	2.17	0.44
3:A:712:TRP:O	3:A:716:LYS:HB3	2.17	0.44
3:A:997:TYR:N	3:A:1003:GLU:HG3	2.24	0.44
3:A:1033:ASN:OD1	3:A:1958:LYS:HD2	2.17	0.44
3:A:1520:ASP:OD2	3:A:1521:LYS:N	2.50	0.44
3:A:1706:ASP:OD1	3:A:1794:GLN:NE2	2.29	0.44
3:A:1972:GLN:O	3:A:1976:ILE:HG13	2.18	0.44
1:B:116:ALA:HB1	1:B:129:LEU:HB3	1.98	0.44
3:A:64:TYR:CE1	3:A:109:ASN:HB2	2.52	0.44
3:A:843:SER:O	3:A:847:GLU:HG2	2.17	0.44
3:A:956:THR:O	3:A:958:TYR:N	2.47	0.44
3:A:975:CYS:SG	3:A:1099:CYS:HA	2.57	0.44
3:A:1201:LYS:NZ	3:A:1207:SER:OG	2.50	0.44
3:A:1946:VAL:HA	3:A:1951:ASP:OD1	2.17	0.44
1:B:230:LYS:HA	1:B:230:LYS:HD3	1.72	0.44
2:C:48:ILE:HA	3:A:510:LYS:HD2	1.99	0.44
3:A:201:TYR:N	3:A:202:PRO:HD3	2.32	0.44
3:A:657:ASP:OD2	3:A:761:ARG:NH2	2.43	0.44
3:A:1000:ASP:HA	3:A:1120:LYS:HD3	2.00	0.44
3:A:1347:VAL:O	3:A:1351:PHE:HB3	2.17	0.44
3:A:589:LEU:HD13	3:A:620:VAL:HG21	1.99	0.44
3:A:1058:ILE:HG21	3:A:1200:LYS:HD3	1.98	0.44
3:A:1130:ASN:OD1	3:A:1131:LYS:N	2.51	0.44
1:B:25:GLU:N	1:B:25:GLU:OE1	2.50	0.44
2:C:111:ASN:CG	2:C:112:ASN:H	2.26	0.44
3:A:34:GLU:HG2	3:A:37:TYR:HE1	1.83	0.44
3:A:150:ASN:N	3:A:238:LYS:HD3	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:184:LYS:HG3	3:A:207:TYR:CE2	2.53	0.44
3:A:940:SER:H	3:A:943:THR:CG2	2.31	0.44
1:B:170:LEU:HA	1:B:208:SER:HA	2.00	0.44
2:C:54:TRP:CE3	2:C:107:CYS:HB3	2.52	0.44
3:A:30:ALA:HB1	3:A:122:ASN:HA	2.00	0.44
3:A:285:GLU:HA	3:A:288:TYR:HB2	1.98	0.44
3:A:366:TYR:CE1	3:A:368:ASP:HB2	2.52	0.44
3:A:993:MET:HG3	3:A:994:LYS:H	1.83	0.44
3:A:1143:ASN:HB3	3:A:1973:LEU:CD2	2.48	0.44
3:A:7:ILE:HG22	3:A:387:TYR:CZ	2.52	0.44
3:A:561:LYS:HB2	3:A:561:LYS:HE3	1.75	0.44
3:A:567:GLU:CD	3:A:567:GLU:N	2.76	0.44
3:A:1635:GLU:O	3:A:1638:PRO:HD2	2.18	0.44
3:A:1755:THR:HG23	3:A:1758:GLN:H	1.83	0.44
2:C:55:TYR:O	2:C:105:TYR:HA	2.18	0.43
3:A:1277:LEU:O	3:A:1287:ASN:HB3	2.18	0.43
3:A:1476:CYS:HB3	3:A:1484:LYS:HG3	2.00	0.43
3:A:1824:PRO:C	3:A:1826:ARG:H	2.25	0.43
1:B:32:ARG:HH21	1:B:142:SER:HA	1.83	0.43
2:C:159:TYR:CG	2:C:160:PRO:HA	2.53	0.43
3:A:561:LYS:CG	3:A:562:LYS:N	2.80	0.43
3:A:659:ILE:O	3:A:708:ARG:NH2	2.45	0.43
3:A:782:ILE:HD13	3:A:960:TYR:CE2	2.53	0.43
3:A:799:CYS:HB2	3:A:802:LYS:CA	2.45	0.43
3:A:945:VAL:O	3:A:945:VAL:HG13	2.18	0.43
3:A:1006:LYS:HZ1	3:A:1011:ASP:HA	1.82	0.43
3:A:1125:GLN:HB3	3:A:1129:ALA:HB3	1.98	0.43
3:A:1408:ILE:C	3:A:1411:GLU:H	2.26	0.43
3:A:1939:PRO:O	3:A:1942:LEU:N	2.33	0.43
1:B:175:PHE:CZ	1:B:176:PRO:HB3	2.53	0.43
3:A:25:ASP:N	3:A:25:ASP:OD1	2.50	0.43
3:A:235:LEU:O	3:A:238:LYS:HG3	2.17	0.43
3:A:251:LYS:HE2	3:A:566:ASN:OD1	2.17	0.43
3:A:288:TYR:OH	3:A:348:LYS:HD3	2.17	0.43
3:A:807:CYS:HB2	3:A:964:CYS:SG	2.59	0.43
3:A:1428:ASN:HB3	3:A:1431:ILE:HD11	2.01	0.43
3:A:1761:TRP:HE1	3:A:1765:GLN:HE21	1.65	0.43
2:C:149:ALA:HB3	2:C:200:LEU:N	2.30	0.43
3:A:97:CYS:HB2	3:A:291:LYS:HD3	1.99	0.43
3:A:181:LYS:HA	3:A:184:LYS:HB2	2.00	0.43
3:A:235:LEU:HA	3:A:258:LYS:CG	2.39	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:629:LYS:HD3	3:A:728:GLU:HG3	2.01	0.43
3:A:1335:ASP:HB2	3:A:1336:PRO:HD2	2.00	0.43
1:B:183:TRP:CH2	1:B:225:CYS:HB3	2.54	0.43
2:C:126:LYS:HA	2:C:159:TYR:OH	2.18	0.43
3:A:231:ARG:HG2	3:A:234:ASP:OD2	2.18	0.43
3:A:334:LYS:C	3:A:338:THR:HB	2.43	0.43
3:A:1268:ARG:NH1	3:A:1350:SER:HA	2.33	0.43
3:A:1305:HIS:CE1	3:A:1427:ASN:HD22	2.36	0.43
3:A:1355:LYS:HA	3:A:1358:ILE:HD12	2.00	0.43
3:A:1526:TYR:CE1	3:A:1538:LEU:HD22	2.54	0.43
3:A:1823:PRO:CB	3:A:1828:ASP:HB2	2.47	0.43
3:A:167:ARG:HG3	3:A:212:GLU:HA	2.01	0.43
3:A:897:PRO:O	3:A:901:LEU:HB2	2.18	0.43
3:A:1136:LYS:HE2	3:A:1140:SER:N	2.30	0.43
3:A:1199:GLU:C	3:A:1201:LYS:N	2.76	0.43
3:A:1227:ILE:HG13	3:A:1299:LYS:HE3	2.00	0.43
3:A:1406:LYS:C	3:A:1409:GLU:H	2.27	0.43
3:A:1866:ILE:HD11	3:A:1880:TYR:CE1	2.54	0.43
3:A:38:TYR:HD2	3:A:59:SER:HA	1.84	0.43
3:A:763:LEU:HD13	3:A:838:ILE:HG21	2.01	0.43
3:A:850:LYS:HE3	3:A:890:ILE:HG21	1.99	0.43
3:A:934:ASP:O	3:A:935:LYS:HB2	2.18	0.43
3:A:1422:LYS:HB3	3:A:1422:LYS:HE3	1.81	0.43
1:B:102:MET:HE2	1:B:105:LEU:HD11	2.01	0.43
1:B:113:TYR:O	1:B:135:GLY:HA2	2.18	0.43
3:A:8:ALA:N	3:A:387:TYR:OH	2.46	0.43
3:A:102:ARG:HA	3:A:105:LEU:HD12	2.01	0.43
3:A:588:TYR:CD2	3:A:620:VAL:HG23	2.54	0.43
3:A:1146:PHE:CD2	3:A:1184:SER:HB3	2.53	0.43
3:A:1297:LYS:HE2	3:A:1297:LYS:HB3	1.87	0.43
3:A:1297:LYS:HG2	3:A:1301:LYS:HE2	2.01	0.43
2:C:147:GLY:HA2	2:C:202:LYS:NZ	2.34	0.43
3:A:35:VAL:HB	3:A:36:GLU:OE1	2.19	0.43
3:A:624:GLU:HB2	3:A:655:TYR:OH	2.19	0.43
3:A:905:LEU:HD23	3:A:905:LEU:HA	1.85	0.43
3:A:982:MET:SD	3:A:982:MET:N	2.92	0.43
3:A:1209:ASP:HA	3:A:1210:THR:HA	1.80	0.43
3:A:1346:ALA:O	3:A:1351:PHE:N	2.37	0.43
1:B:23:LEU:HD22	1:B:53:MET:HE1	2.01	0.42
2:C:166:GLN:NE2	2:C:167:TRP:H	2.17	0.42
3:A:338:THR:HG22	3:A:338:THR:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:564:SER:O	3:A:565:GLY:C	2.62	0.42
3:A:1047:GLU:OE2	3:A:1194:LYS:HE3	2.19	0.42
3:A:1507:LYS:HG3	3:A:1508:TYR:N	2.33	0.42
3:A:1933:CYS:CB	3:A:1934:GLU:HA	2.46	0.42
1:B:48:PHE:CD2	1:B:96:SER:HA	2.54	0.42
2:C:111:ASN:CG	2:C:112:ASN:N	2.77	0.42
2:C:122:ARG:HH2	2:C:161:ARG:HE	1.67	0.42
2:C:199:THR:O	2:C:200:LEU:HD23	2.19	0.42
3:A:69:LYS:HE2	3:A:69:LYS:HB3	1.86	0.42
3:A:604:ASP:OD1	3:A:604:ASP:N	2.52	0.42
3:A:618:LEU:HD13	3:A:722:ALA:HB2	2.00	0.42
3:A:637:ASN:OD1	3:A:638:SER:N	2.52	0.42
3:A:680:ASN:O	3:A:682:GLY:N	2.52	0.42
3:A:862:THR:HG21	3:A:890:ILE:HG13	2.00	0.42
3:A:1164:LYS:HD3	3:A:1972:GLN:NE2	2.34	0.42
3:A:1409:GLU:HA	3:A:1412:MET:H	1.83	0.42
3:A:1584:TYR:CE2	3:A:1769:ARG:HD2	2.54	0.42
3:A:1929:LYS:HA	3:A:1930:GLU:HA	1.62	0.42
1:B:61:GLY:O	1:B:62:LYS:HD2	2.19	0.42
2:C:132:PRO:HB3	2:C:158:PHE:HB3	2.01	0.42
3:A:29:LYS:HA	3:A:218:ASN:ND2	2.34	0.42
3:A:683:LYS:HE3	3:A:683:LYS:HB3	1.68	0.42
3:A:727:ALA:O	3:A:728:GLU:HG3	2.19	0.42
3:A:853:ARG:O	3:A:868:ALA:N	2.52	0.42
3:A:980:GLU:HB2	3:A:981:TYR:CE2	2.54	0.42
3:A:1266:PRO:O	3:A:1270:GLN:HG3	2.19	0.42
3:A:1556:ASN:HB2	3:A:1561:TYR:CD2	2.55	0.42
1:B:120:ARG:HG2	3:A:914:LYS:HB3	2.01	0.42
2:C:174:GLN:HB3	2:C:177:ASN:HD21	1.83	0.42
3:A:101:ARG:HD2	3:A:158:SER:OG	2.19	0.42
3:A:164:ASP:CG	3:A:275:GLN:HB2	2.45	0.42
3:A:325:LYS:O	3:A:329:TYR:CB	2.48	0.42
3:A:344:GLU:HA	3:A:347:TYR:CD2	2.55	0.42
3:A:802:LYS:O	3:A:804:LYS:N	2.52	0.42
3:A:1216:GLU:HB3	3:A:1218:SER:H	1.83	0.42
3:A:1261:ASN:O	3:A:1525:LYS:HG3	2.19	0.42
3:A:1394:VAL:HA	3:A:1397:SER:HB3	2.01	0.42
1:B:37:LEU:HD23	1:B:138:VAL:HG13	2.00	0.42
3:A:81:LYS:HA	3:A:94:GLU:HA	2.01	0.42
3:A:346:LYS:HD3	3:A:346:LYS:N	2.34	0.42
3:A:376:LYS:HA	3:A:381:TYR:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:593:PRO:O	3:A:676:ASN:ND2	2.52	0.42
3:A:689:ILE:HA	3:A:701:TYR:O	2.20	0.42
3:A:731:ILE:HG23	3:A:732:THR:N	2.33	0.42
3:A:850:LYS:NZ	3:A:890:ILE:HG21	2.34	0.42
3:A:857:THR:OG1	3:A:872:THR:HB	2.19	0.42
3:A:1174:GLU:HG2	3:A:1175:PHE:H	1.85	0.42
3:A:1464:GLU:HG3	3:A:1511:TYR:OH	2.19	0.42
3:A:104:ARG:HA	3:A:108:TYR:OH	2.20	0.42
3:A:342:ASN:O	3:A:345:ASN:HB2	2.20	0.42
3:A:497:ASP:HB2	3:A:526:GLU:OE2	2.20	0.42
3:A:610:LYS:N	3:A:684:LEU:HD11	2.35	0.42
3:A:1288:ILE:O	3:A:1288:ILE:HG13	2.20	0.42
3:A:1318:GLY:HA2	3:A:1323:SER:OG	2.20	0.42
3:A:1635:GLU:HB2	3:A:1661:VAL:CG2	2.50	0.42
3:A:1225:ASN:HB2	3:A:1295:LEU:HD21	2.01	0.42
3:A:1307:GLU:O	3:A:1307:GLU:HG3	2.19	0.42
3:A:1914:ALA:O	3:A:1953:LYS:HG3	2.20	0.42
3:A:194:ASP:HB2	3:A:197:LEU:HD11	2.02	0.42
3:A:332:CYS:SG	3:A:335:LYS:HB3	2.59	0.42
3:A:344:GLU:OE2	3:A:348:LYS:HE2	2.20	0.42
3:A:380:ASN:OD1	3:A:381:TYR:N	2.52	0.42
3:A:529:LYS:HG3	3:A:530:LYS:N	2.30	0.42
3:A:684:LEU:C	3:A:686:GLY:H	2.28	0.42
3:A:798:GLU:HB2	3:A:966:CYS:SG	2.60	0.42
3:A:853:ARG:O	3:A:869:ALA:N	2.43	0.42
3:A:949:VAL:O	3:A:949:VAL:HG13	2.20	0.42
3:A:1397:SER:OG	3:A:1398:THR:N	2.53	0.42
3:A:1409:GLU:O	3:A:1413:TRP:HB2	2.20	0.42
3:A:1981:LYS:HE2	3:A:1988:LEU:HD23	2.01	0.42
2:C:155:LEU:HB2	2:C:194:LEU:HB3	2.02	0.42
3:A:7:ILE:HG12	3:A:7:ILE:O	2.19	0.42
3:A:8:ALA:H	3:A:387:TYR:HH	1.67	0.42
3:A:279:TRP:HA	3:A:282:GLU:HB3	2.02	0.42
3:A:1125:GLN:HB3	3:A:1129:ALA:HB2	2.01	0.42
3:A:1125:GLN:CA	3:A:1128:ASP:H	2.27	0.42
3:A:1195:LEU:C	3:A:1198:ALA:H	2.28	0.42
3:A:1300:ILE:HD13	3:A:1351:PHE:CE1	2.54	0.42
3:A:1484:LYS:HG2	3:A:1573:ILE:O	2.19	0.42
3:A:1558:ASN:CG	3:A:1560:GLU:HG2	2.44	0.42
1:B:50:ASP:HA	1:B:72:TRP:HB2	2.02	0.42
3:A:39:ARG:HG2	3:A:115:PHE:CE2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:928:LYS:HG3	3:A:931:LYS:O	2.20	0.42
3:A:1106:LYS:HB3	3:A:1106:LYS:HE3	1.75	0.42
3:A:1129:ALA:HA	3:A:1132:GLY:H	1.85	0.42
3:A:1308:THR:HA	3:A:1311:LEU:H	1.85	0.42
3:A:1315:HIS:HA	3:A:1323:SER:HB3	2.02	0.42
3:A:1833:ASN:CB	3:A:1838:CYS:HB3	2.50	0.42
3:A:1839:LYS:HD3	3:A:1968:HIS:HB2	2.02	0.42
3:A:274:PRO:HG2	3:A:373:PHE:CE2	2.55	0.41
3:A:1919:SER:HA	3:A:1920:GLY:HA2	1.49	0.41
2:C:58:LYS:NZ	2:C:100:GLU:O	2.37	0.41
3:A:365:ARG:NH1	3:A:374:PHE:HB2	2.23	0.41
3:A:688:TYR:O	3:A:700:SER:HB2	2.20	0.41
3:A:858:LYS:C	3:A:858:LYS:HD2	2.45	0.41
3:A:995:ARG:NH1	3:A:997:TYR:OH	2.53	0.41
3:A:1124:LYS:O	3:A:1128:ASP:N	2.53	0.41
3:A:1696:TYR:CD1	3:A:1791:ALA:HB2	2.54	0.41
3:A:1988:LEU:CG	3:A:1989:ASP:H	2.30	0.41
3:A:67:CYS:HA	3:A:108:TYR:HD2	1.85	0.41
3:A:236:LEU:HD22	3:A:260:GLY:H	1.85	0.41
3:A:342:ASN:HA	3:A:345:ASN:ND2	2.36	0.41
3:A:986:SER:HA	3:A:993:MET:HB3	2.02	0.41
3:A:1311:LEU:O	3:A:1316:ASP:N	2.53	0.41
3:A:1365:ILE:O	3:A:1365:ILE:HG23	2.20	0.41
3:A:1649:LYS:HA	3:A:1652:GLU:CD	2.44	0.41
1:B:179:VAL:HG12	1:B:229:HIS:HA	2.03	0.41
3:A:975:CYS:SG	3:A:1102:LEU:HD23	2.60	0.41
3:A:1617:ARG:HD3	3:A:1617:ARG:HA	1.72	0.41
3:A:1922:VAL:HG23	3:A:1922:VAL:O	2.20	0.41
3:A:339:GLU:HA	3:A:343:GLN:CB	2.50	0.41
3:A:1377:LYS:HA	3:A:1381:GLU:CD	2.45	0.41
3:A:1469:GLU:O	3:A:1473:ARG:HG2	2.20	0.41
3:A:1741:TRP:O	3:A:1746:THR:OG1	2.35	0.41
3:A:1761:TRP:NE1	3:A:1765:GLN:HE21	2.19	0.41
3:A:65:ASP:O	3:A:109:ASN:HB3	2.21	0.41
3:A:559:ILE:C	3:A:561:LYS:N	2.74	0.41
3:A:1041:GLU:OE1	3:A:1853:ARG:NH2	2.52	0.41
3:A:1097:CYS:HA	3:A:1101:LYS:HE3	2.03	0.41
3:A:1197:ASN:C	3:A:1199:GLU:N	2.78	0.41
3:A:1201:LYS:HD3	3:A:1201:LYS:HA	1.76	0.41
3:A:1626:PRO:HA	3:A:1629:GLN:HG2	2.02	0.41
2:C:23:MET:HE3	2:C:42:CYS:SG	2.61	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:7:ILE:HG13	3:A:376:LYS:HB2	2.02	0.41
3:A:97:CYS:HB2	3:A:291:LYS:CE	2.51	0.41
3:A:344:GLU:HA	3:A:347:TYR:CB	2.45	0.41
3:A:365:ARG:HH21	3:A:370:VAL:HG22	1.85	0.41
3:A:687:LYS:HD2	3:A:688:TYR:CD2	2.55	0.41
3:A:1420:ILE:HA	3:A:1423:ILE:HD12	2.02	0.41
3:A:1572:SER:O	3:A:1642:LYS:HD2	2.20	0.41
3:A:1698:LEU:HD12	3:A:1698:LEU:HA	1.84	0.41
3:A:1978:ASN:HA	3:A:1981:LYS:HG2	2.02	0.41
1:B:174:TYR:OH	1:B:207:LEU:HD23	2.21	0.41
1:B:185:SER:H	1:B:226:ASN:ND2	2.19	0.41
3:A:284:ILE:O	3:A:287:PHE:HB3	2.21	0.41
3:A:287:PHE:O	3:A:288:TYR:C	2.63	0.41
3:A:1136:LYS:CE	3:A:1140:SER:H	2.31	0.41
3:A:1227:ILE:HD13	3:A:1276:GLU:OE2	2.20	0.41
3:A:1276:GLU:O	3:A:1287:ASN:ND2	2.53	0.41
3:A:1317:THR:HA	3:A:1330:GLN:NE2	2.35	0.41
1:B:175:PHE:CE2	1:B:176:PRO:HB3	2.56	0.41
2:C:108:GLN:HG3	2:C:117:PHE:CZ	2.55	0.41
2:C:169:VAL:HG13	2:C:211:TYR:HE1	1.86	0.41
3:A:25:ASP:O	3:A:29:LYS:HG3	2.21	0.41
3:A:109:ASN:OD1	3:A:110:LEU:N	2.52	0.41
3:A:111:GLU:HG2	3:A:179:LEU:HD22	2.03	0.41
3:A:236:LEU:CB	3:A:260:GLY:H	2.34	0.41
3:A:412:ASN:HB3	3:A:413:PRO:HD2	2.02	0.41
3:A:533:LYS:HB3	3:A:534:VAL:H	1.65	0.41
3:A:698:ASP:N	3:A:699:THR:CB	2.81	0.41
3:A:720:TRP:NE1	3:A:724:LYS:HE2	2.35	0.41
3:A:925:THR:N	3:A:946:VAL:N	2.66	0.41
3:A:925:THR:O	3:A:926:THR:C	2.62	0.41
3:A:951:SER:C	3:A:953:LEU:H	2.24	0.41
3:A:1012:VAL:HG23	3:A:1950:MET:HE1	2.02	0.41
3:A:1019:SER:OG	3:A:1026:GLY:HA2	2.21	0.41
3:A:1049:TYR:O	3:A:1053:ALA:HA	2.19	0.41
3:A:1058:ILE:HA	3:A:1059:ASP:HA	1.67	0.41
3:A:1174:GLU:O	3:A:1177:ILE:HG13	2.21	0.41
3:A:1221:LEU:HB3	3:A:1224:THR:HA	2.02	0.41
3:A:1379:ILE:O	3:A:1382:LYS:HG2	2.21	0.41
1:B:46:PHE:CE1	1:B:117:ARG:NE	2.88	0.41
2:C:55:TYR:CE1	2:C:108:GLN:HB3	2.56	0.41
2:C:201:SER:O	2:C:205:TYR:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1029:VAL:HG21	3:A:1959:MET:CE	2.50	0.41
3:A:1355:LYS:O	3:A:1358:ILE:HB	2.21	0.41
3:A:1436:GLU:H	3:A:1436:GLU:CD	2.27	0.41
3:A:1588:GLU:HG2	3:A:1770:TYR:OH	2.21	0.41
3:A:1933:CYS:HB2	3:A:1935:GLU:HA	2.03	0.41
2:C:23:MET:HE3	2:C:23:MET:HB3	2.00	0.40
2:C:34:ILE:HD12	2:C:34:ILE:H	1.85	0.40
3:A:34:GLU:OE1	3:A:34:GLU:N	2.55	0.40
3:A:334:LYS:HA	3:A:338:THR:OG1	2.21	0.40
3:A:1247:LYS:HD2	3:A:1271:ASN:HB3	2.03	0.40
1:B:70:ILE:HG13	1:B:77:LYS:HG2	2.03	0.40
2:C:109:LYS:HZ1	2:C:114:PRO:HD2	1.86	0.40
3:A:156:GLU:OE1	3:A:270:LEU:HD22	2.21	0.40
3:A:529:LYS:HE3	3:A:718:TYR:CZ	2.56	0.40
3:A:1322:ILE:H	3:A:1322:ILE:HD12	1.86	0.40
3:A:1663:GLU:HB2	3:A:1763:ALA:HB1	2.04	0.40
3:A:1884:MET:O	3:A:1884:MET:HG2	2.20	0.40
3:A:1912:ILE:HG12	3:A:1913:GLY:N	2.37	0.40
3:A:853:ARG:HH22	3:A:866:THR:HG22	1.86	0.40
3:A:1294:GLU:O	3:A:1297:LYS:HB3	2.22	0.40
3:A:1313:GLU:HA	3:A:1317:THR:HG23	2.03	0.40
3:A:1612:LYS:HB2	3:A:1612:LYS:HE2	1.68	0.40
3:A:1827:ALA:O	3:A:1828:ASP:C	2.64	0.40
3:A:1943:MET:HA	3:A:1946:VAL:HG12	2.03	0.40
3:A:277:LEU:HD13	3:A:373:PHE:CE1	2.56	0.40
3:A:560:TRP:HH2	3:A:838:ILE:HG13	1.87	0.40
3:A:584:THR:O	3:A:587:LEU:HG	2.22	0.40
3:A:731:ILE:HG23	3:A:732:THR:H	1.85	0.40
3:A:1045:GLN:NE2	3:A:1049:TYR:CD2	2.90	0.40
3:A:1109:ASP:O	3:A:1113:LYS:HG2	2.22	0.40
3:A:1424:ASN:O	3:A:1431:ILE:HG12	2.21	0.40
3:A:1596:CYS:HB2	3:A:1668:TYR:CD2	2.56	0.40
3:A:1695:PHE:HB2	3:A:1764:MET:HE3	2.01	0.40
3:A:1697:ASP:O	3:A:1701:ILE:HG13	2.22	0.40
3:A:344:GLU:C	3:A:346:LYS:N	2.79	0.40
3:A:496:GLN:HB3	3:A:497:ASP:H	1.74	0.40
3:A:925:THR:O	3:A:946:VAL:CG1	2.70	0.40
3:A:1296:LEU:O	3:A:1300:ILE:HG13	2.22	0.40
3:A:1688:CYS:O	3:A:1692:ARG:HG2	2.22	0.40
3:A:1966:LEU:HD13	3:A:1966:LEU:HA	1.79	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	B	219/472 (46%)	205 (94%)	14 (6%)	0	100	100
2	C	210/233 (90%)	189 (90%)	21 (10%)	0	100	100
3	A	1843/2040 (90%)	1512 (82%)	305 (16%)	26 (1%)	9	36
All	All	2272/2745 (83%)	1906 (84%)	340 (15%)	26 (1%)	14	43

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	563	SER
3	A	566	ASN
3	A	683	LYS
3	A	690	LYS
3	A	699	THR
3	A	966	CYS
3	A	967	LYS
3	A	533	LYS
3	A	561	LYS
3	A	564	SER
3	A	695	ALA
3	A	512	GLY
3	A	525	ASP
3	A	556	LYS
3	A	571	GLN
3	A	687	LYS
3	A	688	TYR
3	A	691	LYS
3	A	702	SER
3	A	93	PRO
3	A	350	LEU
3	A	514	SER
3	A	965	GLN
3	A	906	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	237	ILE
3	A	682	GLY

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	B	181/411 (44%)	180 (99%)	1 (1%)	78	88
2	C	184/201 (92%)	184 (100%)	0	100	100
3	A	1674/1839 (91%)	1647 (98%)	27 (2%)	55	79
All	All	2039/2451 (83%)	2011 (99%)	28 (1%)	57	80

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	22	ARG
3	A	7	ILE
3	A	118	ILE
3	A	198	GLN
3	A	514	SER
3	A	555	LYS
3	A	556	LYS
3	A	557	LYS
3	A	559	ILE
3	A	561	LYS
3	A	562	LYS
3	A	567	GLU
3	A	568	GLU
3	A	683	LYS
3	A	687	LYS
3	A	689	ILE
3	A	690	LYS
3	A	691	LYS
3	A	693	ASN
3	A	694	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	696	GLU
3	A	699	THR
3	A	700	SER
3	A	867	ASN
3	A	890	ILE
3	A	1365	ILE
3	A	1912	ILE
3	A	1980	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	184	ASN
3	A	84	GLN
3	A	147	ASN
3	A	185	GLN
3	A	310	HIS
3	A	345	ASN
3	A	354	ASN
3	A	360	GLN
3	A	509	ASN
3	A	693	ASN
3	A	697	GLN
3	A	769	ASN
3	A	773	GLN
3	A	859	ASN
3	A	879	GLN
3	A	1008	ASN
3	A	1033	ASN
3	A	1039	ASN
3	A	1114	GLN
3	A	1305	HIS
3	A	1315	HIS
3	A	1348	GLN
3	A	1356	ASN
3	A	1427	ASN
3	A	1517	GLN
3	A	1522	GLN
3	A	1601	ASN
3	A	1674	ASN
3	A	1765	GLN
3	A	1787	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	1864	ASN
3	A	1957	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

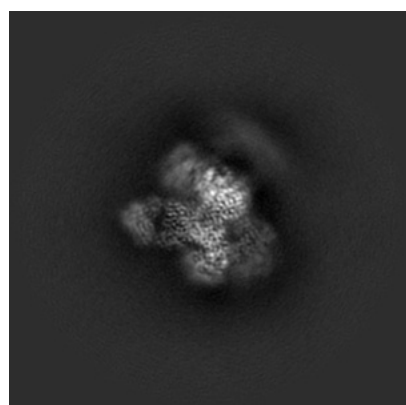
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14438. These allow visual inspection of the internal detail of the map and identification of artifacts.

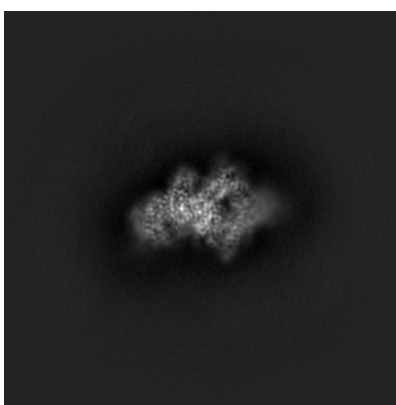
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

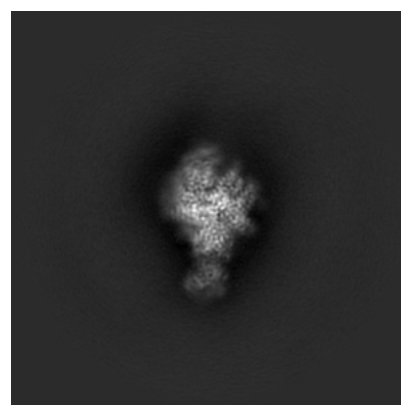
6.1.1 Primary map



X



Y

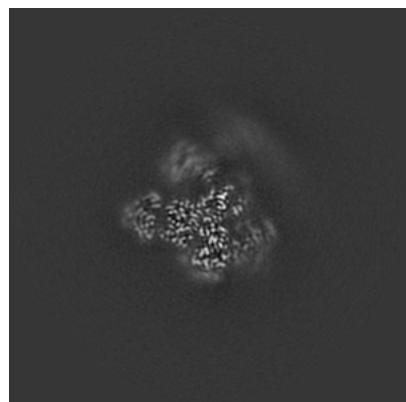


Z

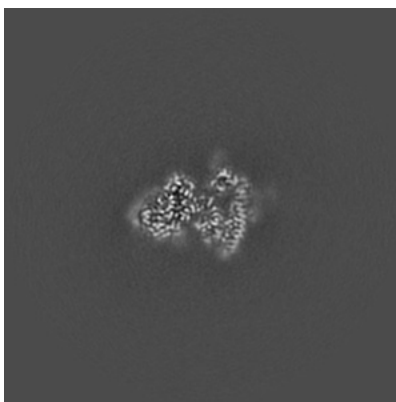
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

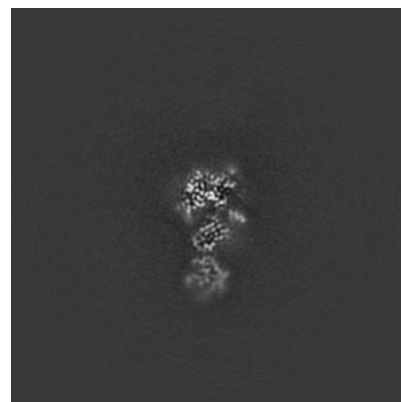
6.2.1 Primary map



X Index: 220



Y Index: 220

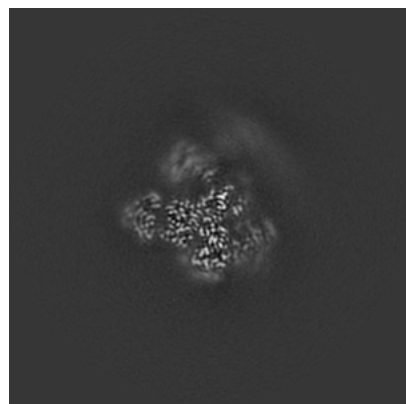


Z Index: 220

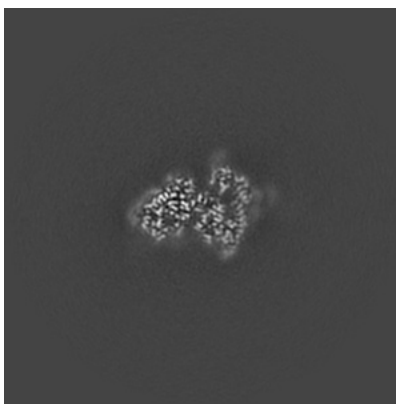
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

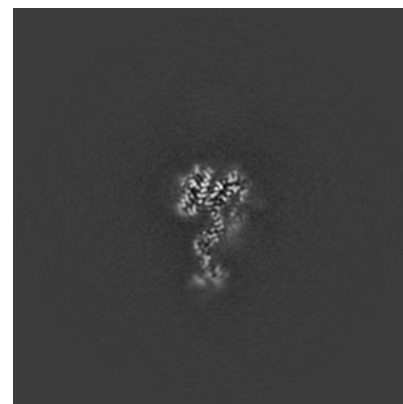
6.3.1 Primary map



X Index: 220



Y Index: 223

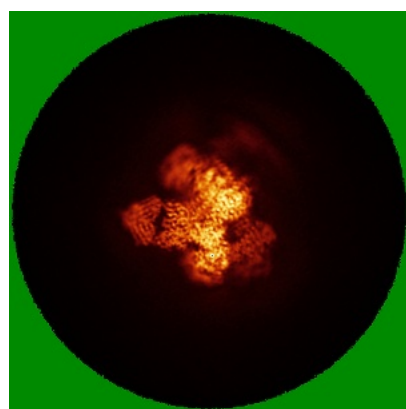


Z Index: 225

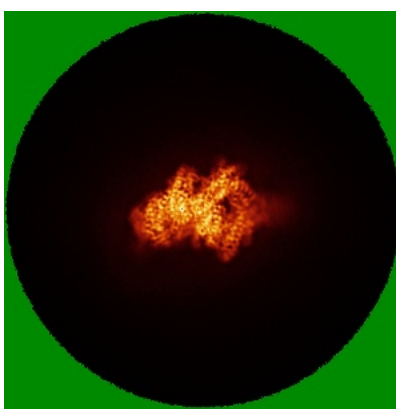
The images above show the largest variance slices of the map in three orthogonal directions.

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

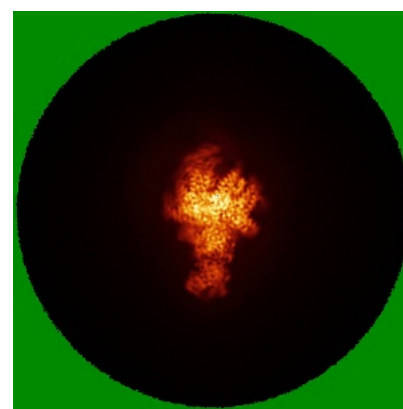
6.4.1 Primary map



X



Y

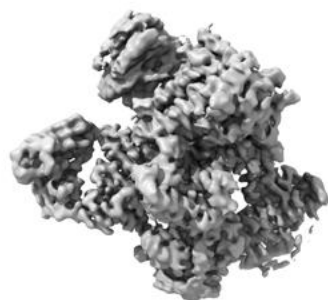


Z

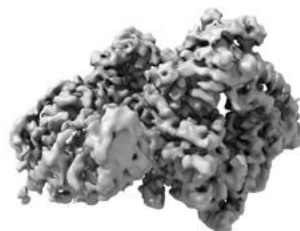
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

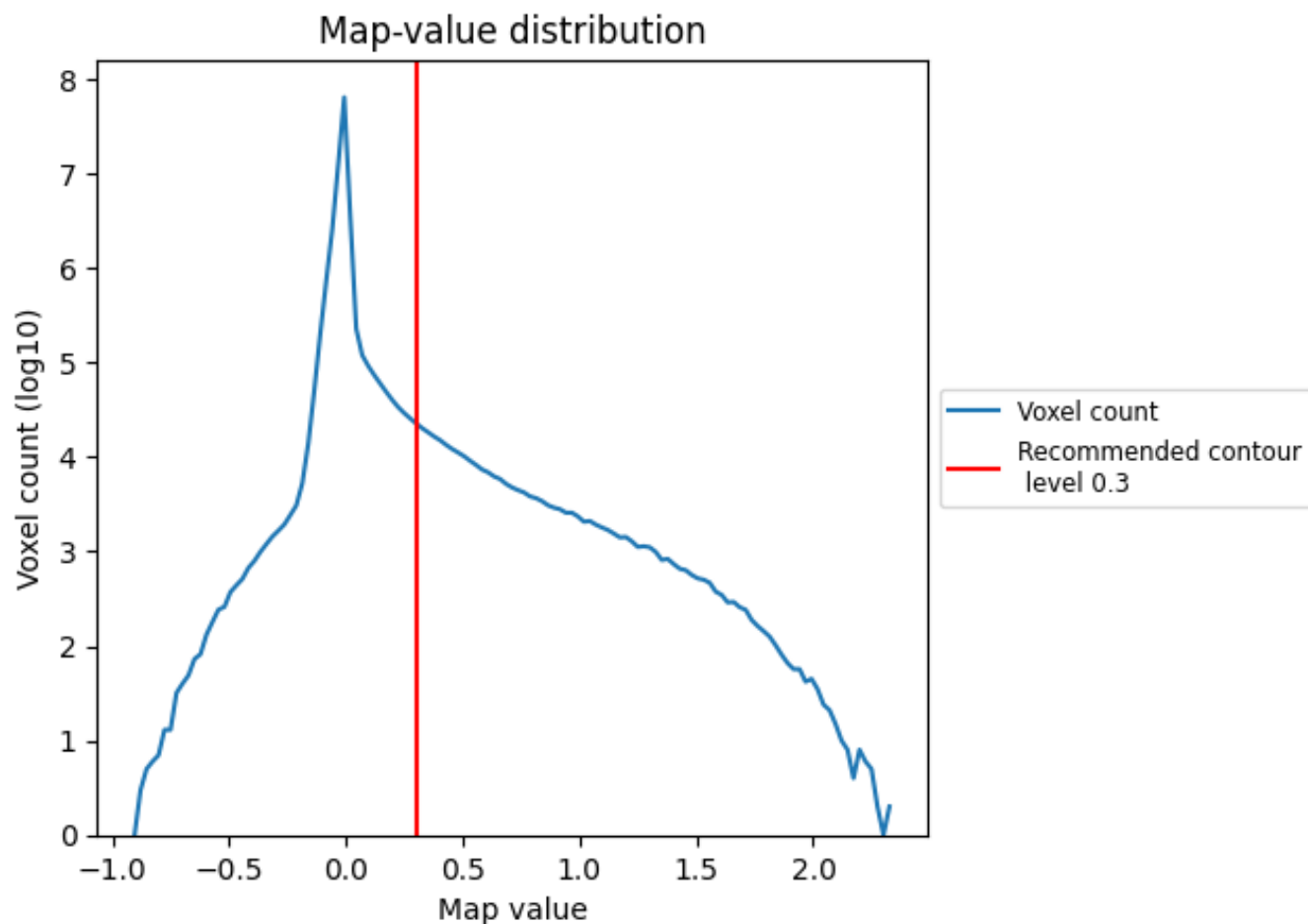
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

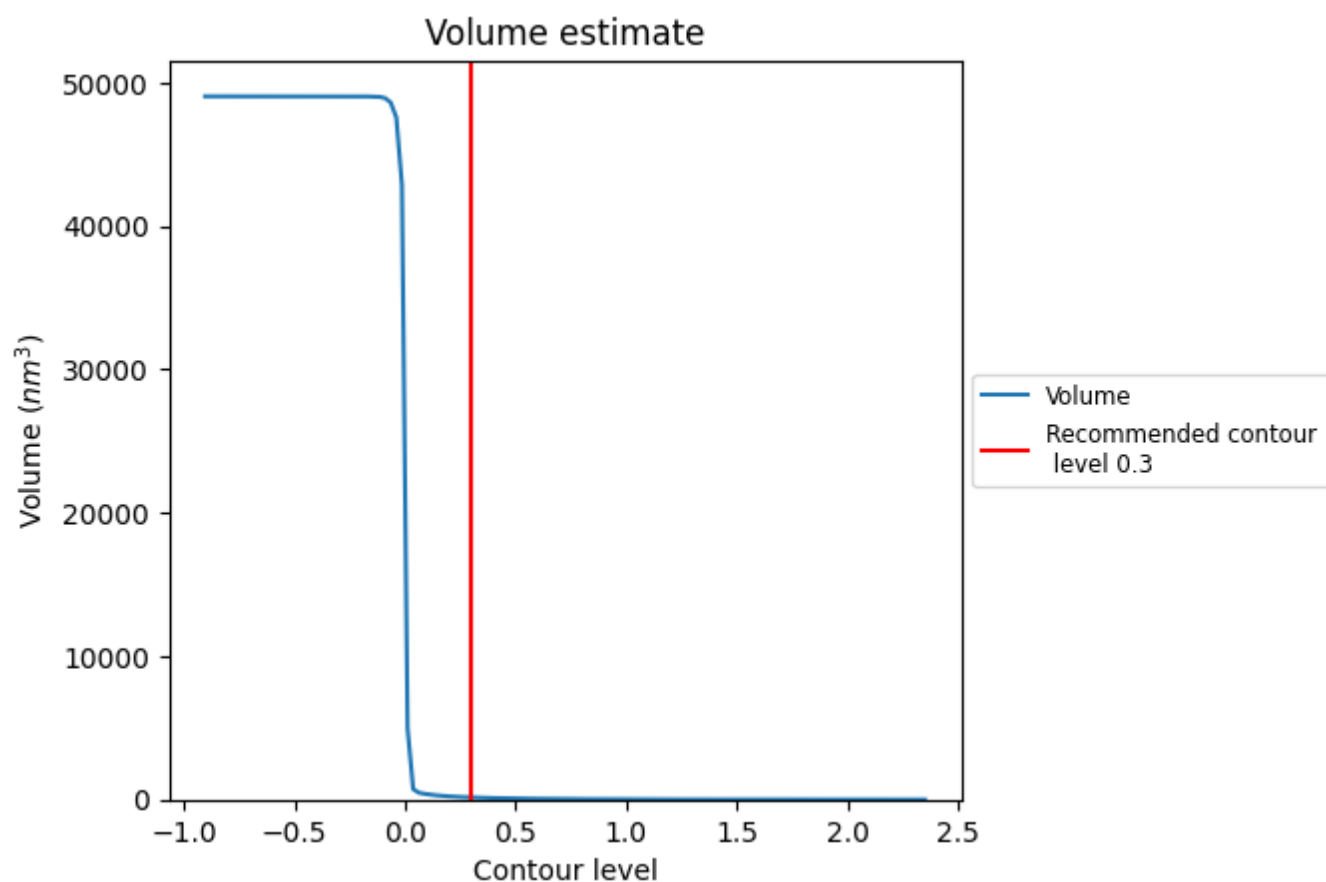
This section contains the results of statistical analysis of the map.

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.

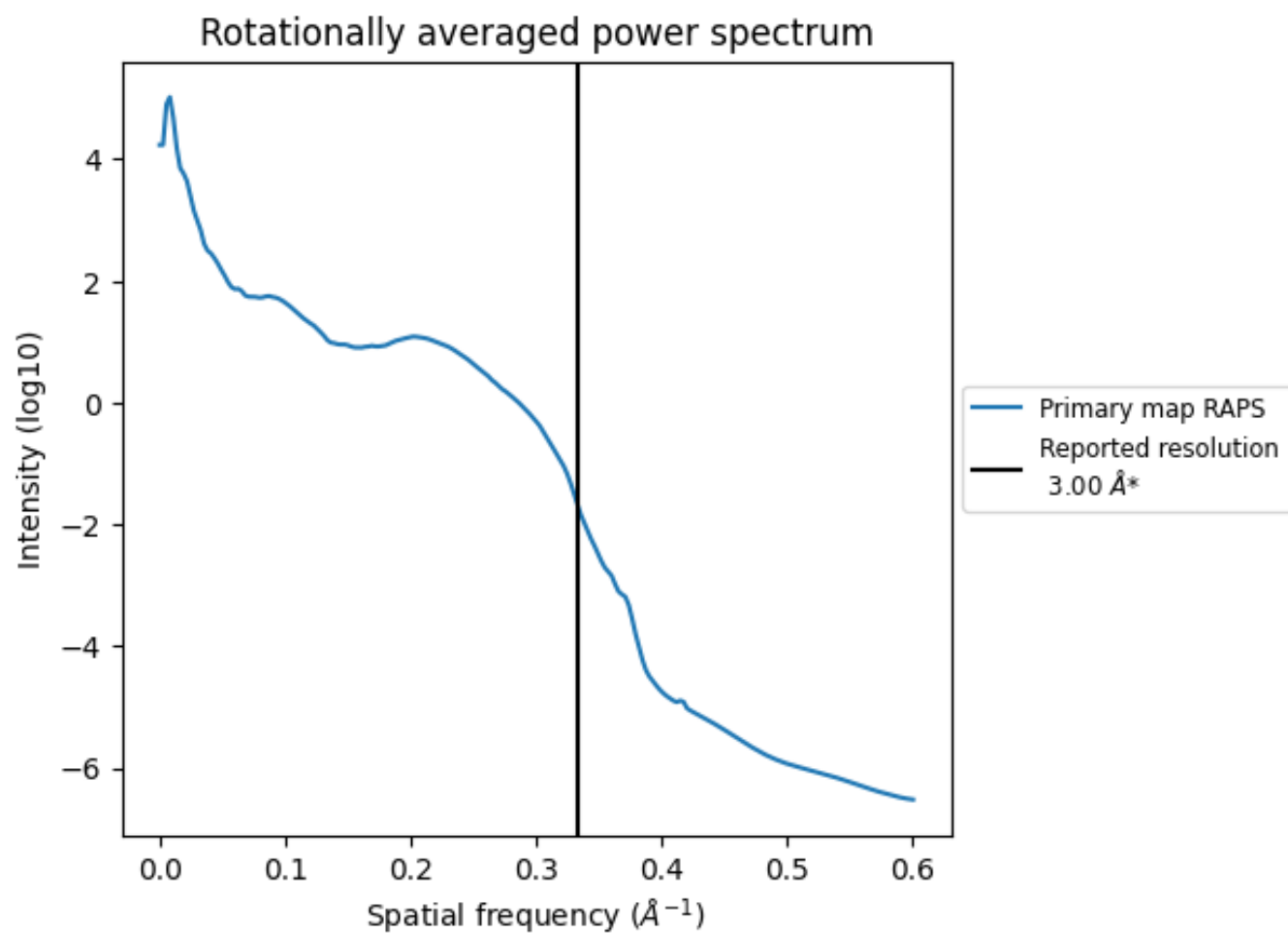
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 149 nm³; this corresponds to an approximate mass of 134 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 ⓘ

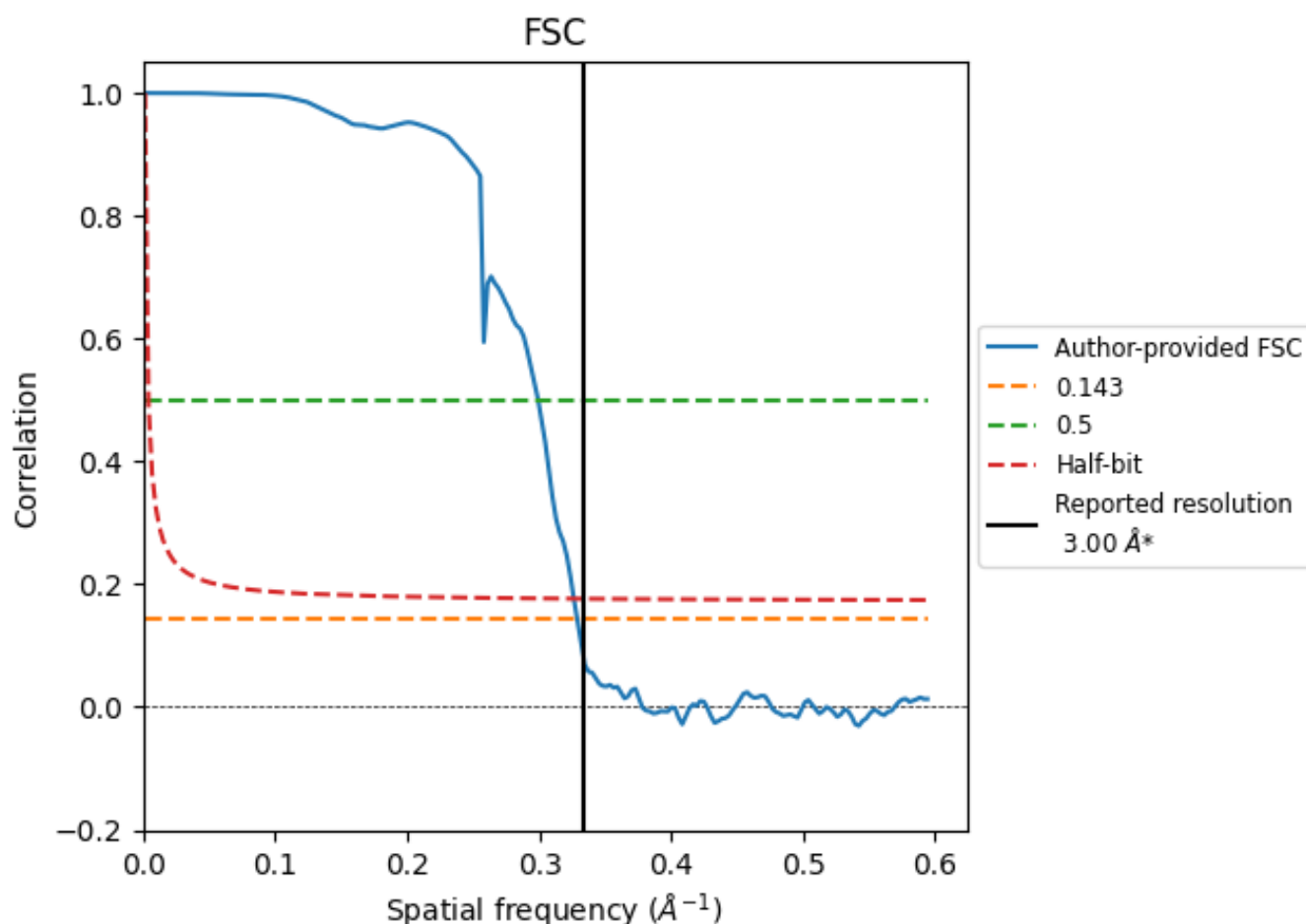


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

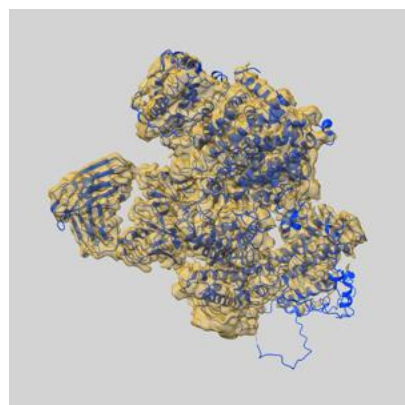
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.04	3.34	3.06
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

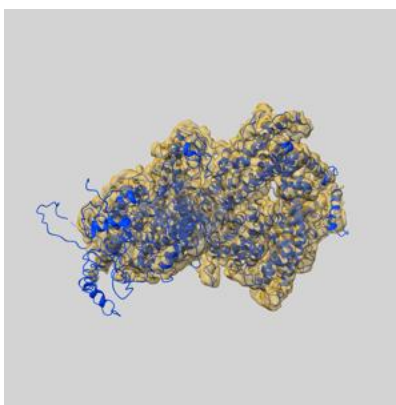
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14438 and PDB model 7Z12. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

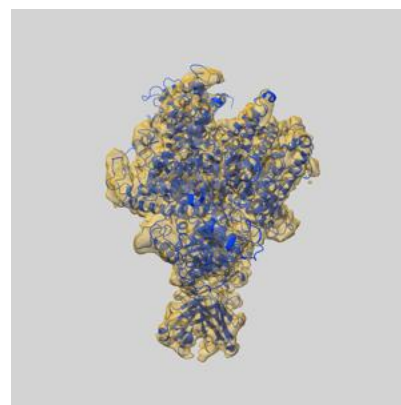
9.1 Map-model overlay [i](#)



X



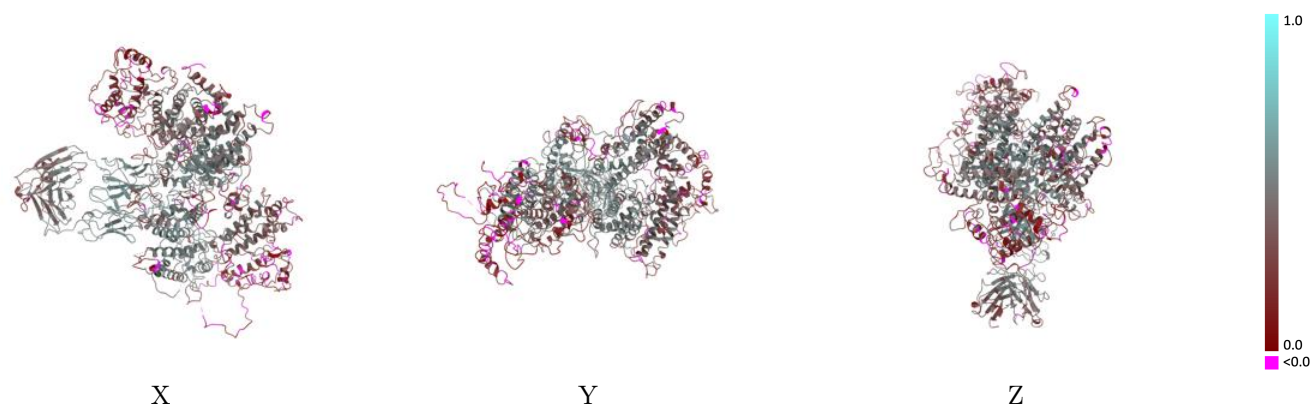
Y



Z

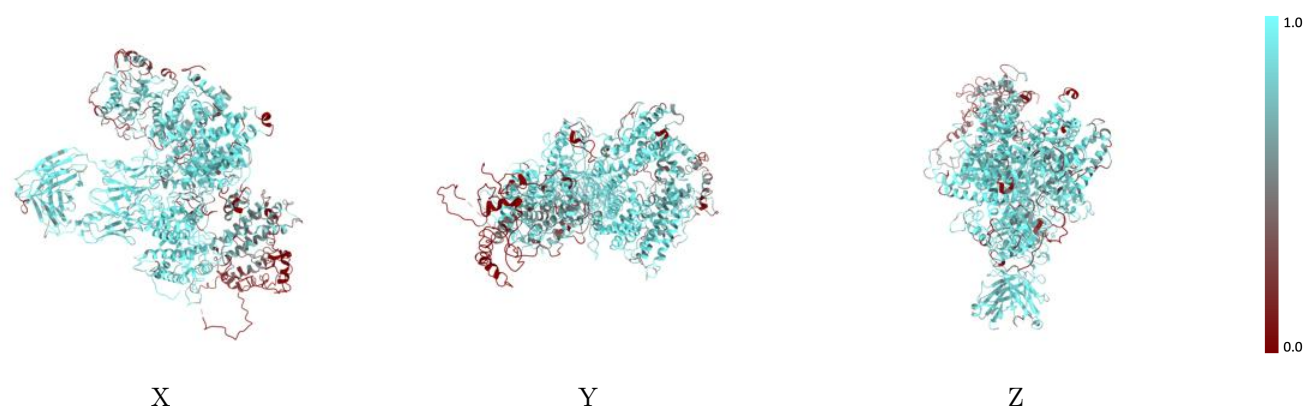
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



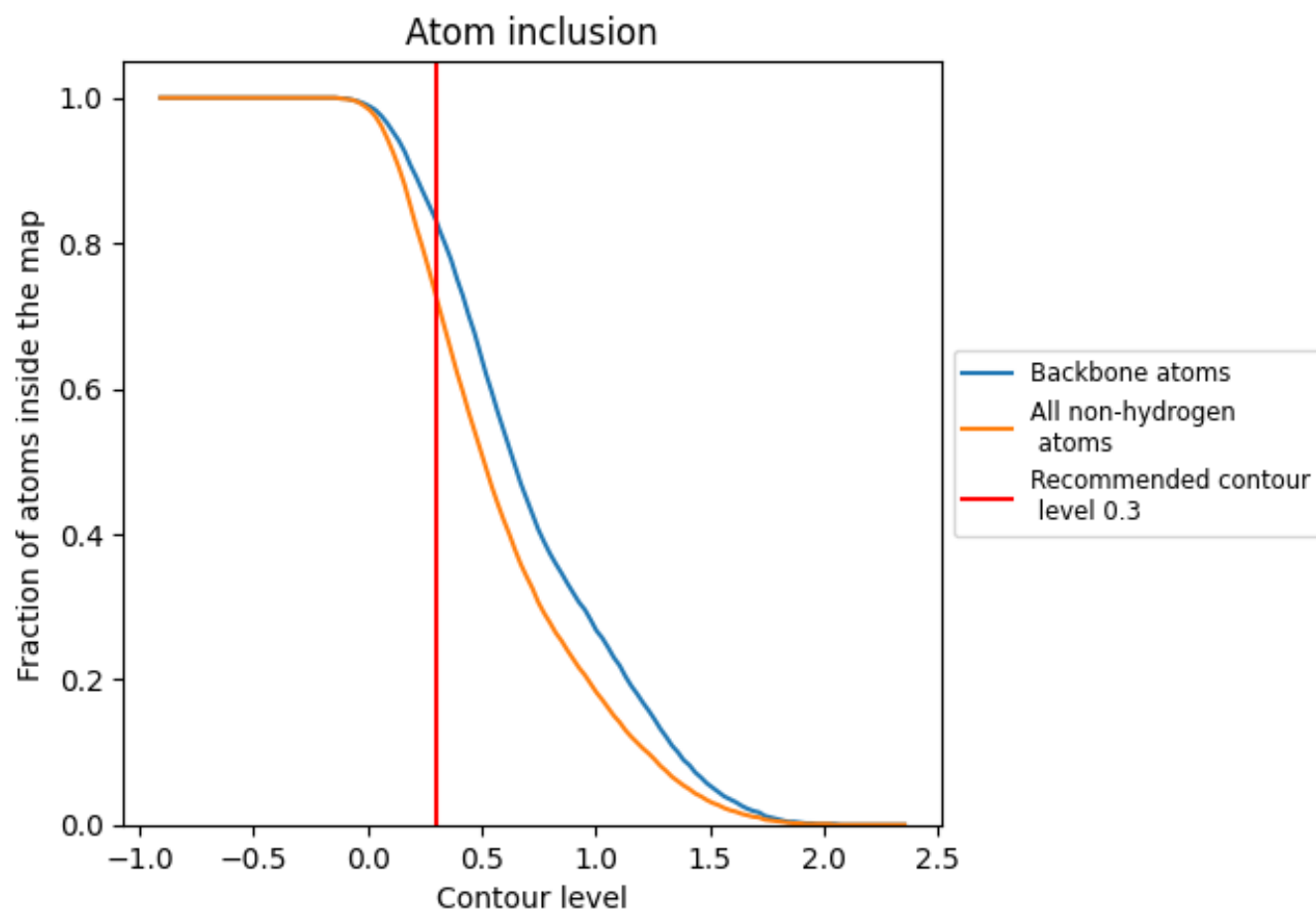
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion ⓘ



At the recommended contour level, 83% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7280	0.3620
A	0.6940	0.3360
B	0.8900	0.4880
C	0.8770	0.4750

