Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 03:30 PM JST

PDB ID	:	6J8I
EMDB ID	:	EMD-9782
Title	:	Structure of human voltage-gated sodium channel Nav1.7 in complex with auxiliary beta subunits, ProTx-II and tetrodotoxin (Y1755 up)
Authors	:	Shen, H.; Liu, D.; Lei, J.; Yan, N.
Deposited on	:	2019-01-19
Resolution	:	3.20 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:

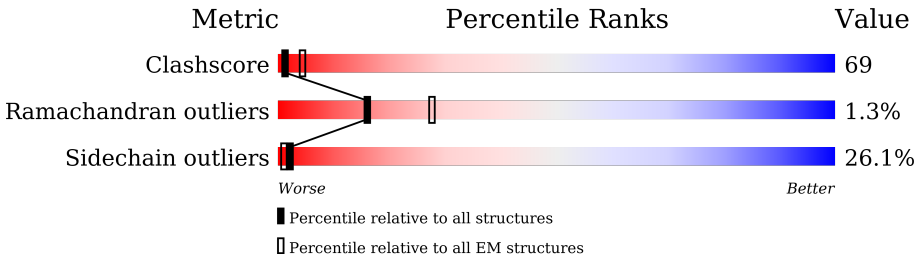
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	C	215	51% 30% 20% 5% 44%
2	A	2031	8% 19% 27% 10% 44%
3	B	218	5% 22% 39% 17% 21%
4	D	2	100%
4	E	2	50% 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	C	301	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11764 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 Sodium channel subunit beta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	120	Total	C	N	O	S	0	0
			980	614	173	182	11		

- Molecule 2 is a protein called Sodium channel protein type 9 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1140	Total	C	N	O	S	0	0
			9192	6110	1438	1568	76		

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	MET	-	expression tag	UNP Q15858
A	-41	ALA	-	expression tag	UNP Q15858
A	-40	SER	-	expression tag	UNP Q15858
A	-39	TRP	-	expression tag	UNP Q15858
A	-38	SER	-	expression tag	UNP Q15858
A	-37	HIS	-	expression tag	UNP Q15858
A	-36	PRO	-	expression tag	UNP Q15858
A	-35	GLN	-	expression tag	UNP Q15858
A	-34	PHE	-	expression tag	UNP Q15858
A	-33	GLU	-	expression tag	UNP Q15858
A	-32	LYS	-	expression tag	UNP Q15858
A	-31	GLY	-	expression tag	UNP Q15858
A	-30	GLY	-	expression tag	UNP Q15858
A	-29	GLY	-	expression tag	UNP Q15858
A	-28	ALA	-	expression tag	UNP Q15858
A	-27	ARG	-	expression tag	UNP Q15858
A	-26	GLY	-	expression tag	UNP Q15858
A	-25	GLY	-	expression tag	UNP Q15858
A	-24	SER	-	expression tag	UNP Q15858
A	-23	GLY	-	expression tag	UNP Q15858
A	-22	GLY	-	expression tag	UNP Q15858

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	GLY	-	expression tag	UNP Q15858
A	-20	SER	-	expression tag	UNP Q15858
A	-19	TRP	-	expression tag	UNP Q15858
A	-18	SER	-	expression tag	UNP Q15858
A	-17	HIS	-	expression tag	UNP Q15858
A	-16	PRO	-	expression tag	UNP Q15858
A	-15	GLN	-	expression tag	UNP Q15858
A	-14	PHE	-	expression tag	UNP Q15858
A	-13	GLU	-	expression tag	UNP Q15858
A	-12	LYS	-	expression tag	UNP Q15858
A	-11	GLY	-	expression tag	UNP Q15858
A	-10	PHE	-	expression tag	UNP Q15858
A	-9	ASP	-	expression tag	UNP Q15858
A	-8	TYR	-	expression tag	UNP Q15858
A	-7	LYS	-	expression tag	UNP Q15858
A	-6	ASP	-	expression tag	UNP Q15858
A	-5	ASP	-	expression tag	UNP Q15858
A	-4	ASP	-	expression tag	UNP Q15858
A	-3	ASP	-	expression tag	UNP Q15858
A	-2	LYS	-	expression tag	UNP Q15858
A	-1	GLY	-	expression tag	UNP Q15858
A	0	THR	-	expression tag	UNP Q15858
A	406	LYS	GLU	variant	UNP Q15858

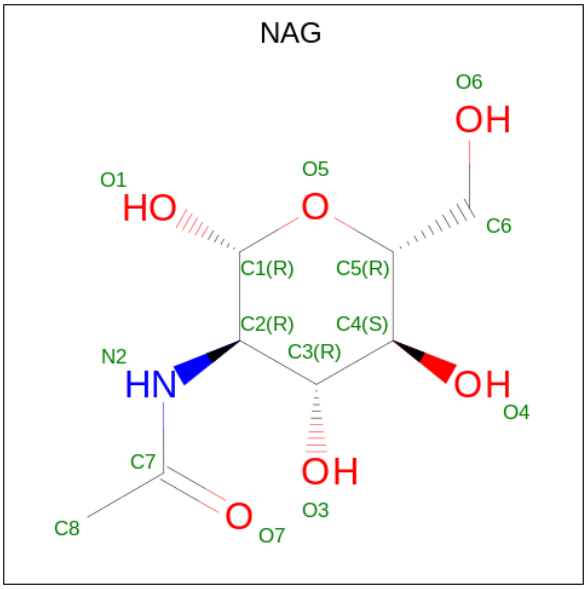
- Molecule 3 is a protein called Sodium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	173	Total	C	N	O	S	0	0
			1416	902	232	272	10		

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

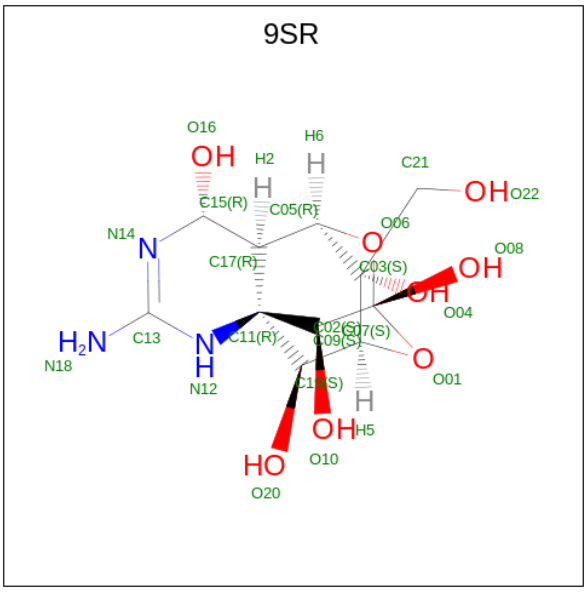
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
5	C	1	Total C N O 14 8 1 5	0
5	A	1	Total C N O 28 16 2 10	0
5	A	1	Total C N O 28 16 2 10	0
5	B	1	Total C N O 56 32 4 20	0
5	B	1	Total C N O 56 32 4 20	0
5	B	1	Total C N O 56 32 4 20	0
5	B	1	Total C N O 56 32 4 20	0

- Molecule 6 is (1R,5R,6R,7R,9S,11S,12S,13S,14S)-3-amino-14-(hydroxymethyl)-8,10-dioxa-2,4-diazatetracyclo[7.3.1.1 7,11 .0 1,6]tetradec-3-ene-5,9,12,13,14-pentol (non-preferred name) (three-letter code: 9SR) (formula: $C_{11}H_{17}N_3O_8$).

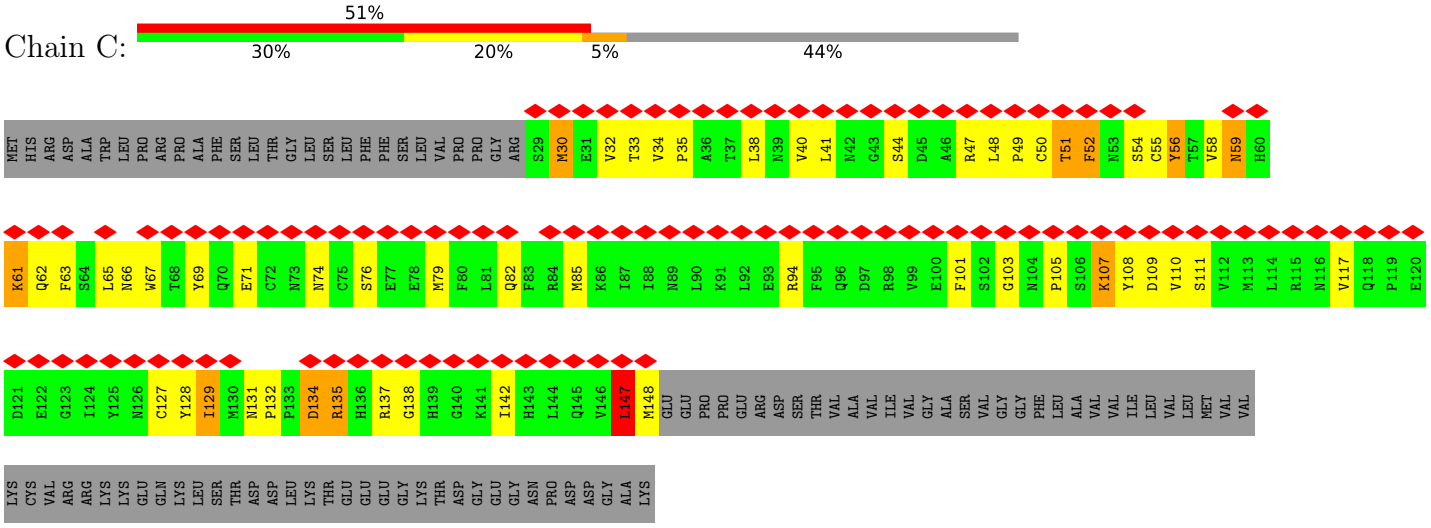


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	A	1	22	11	3	8	0

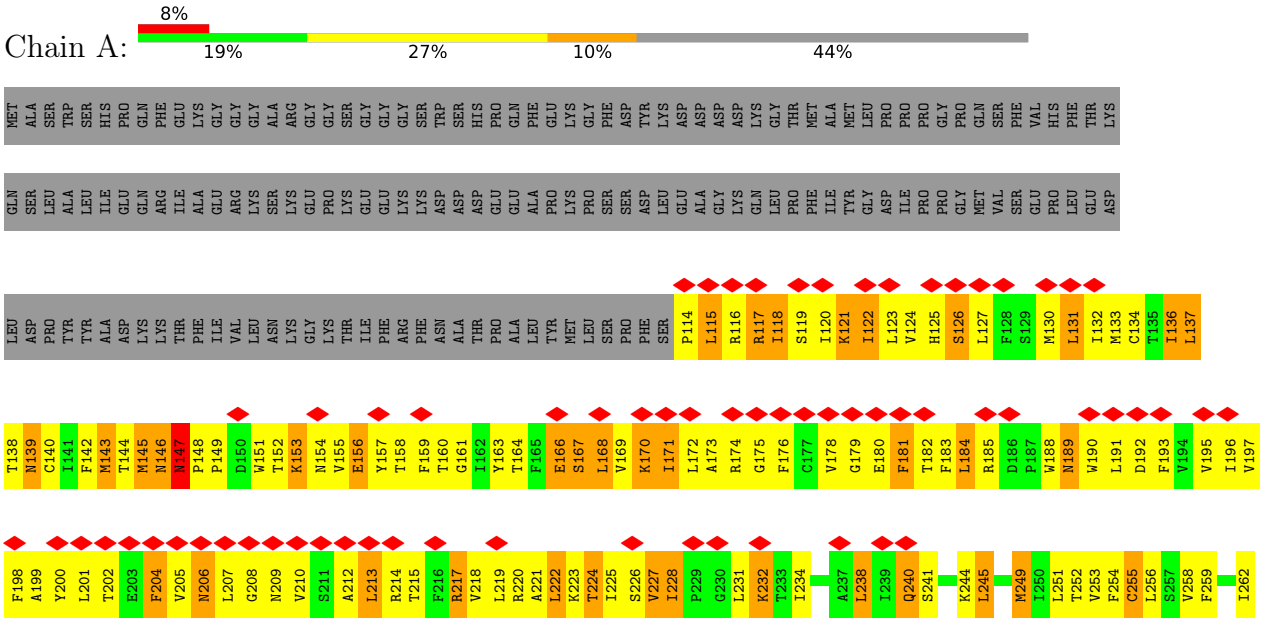
3 Residue-property plots (i)

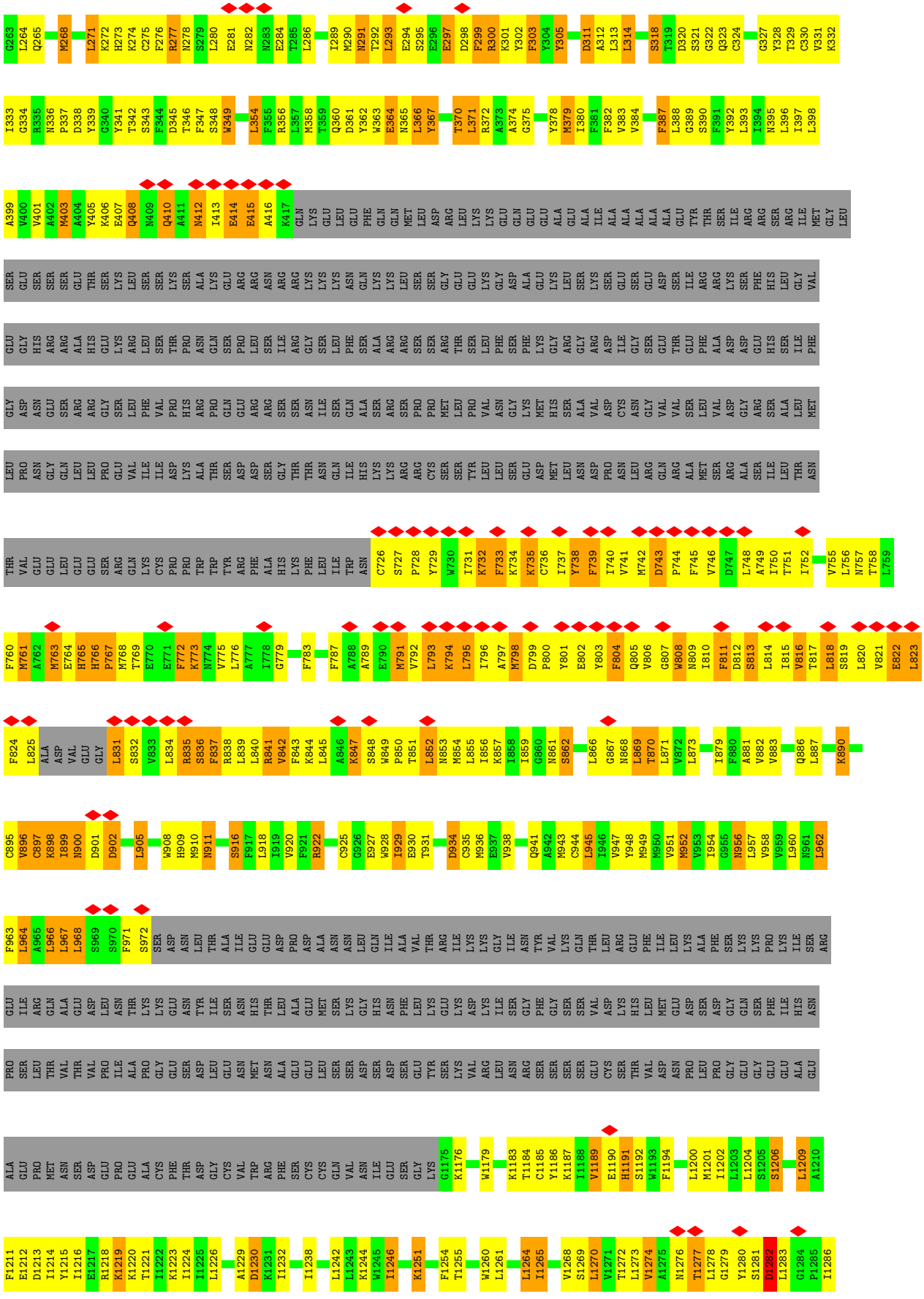
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

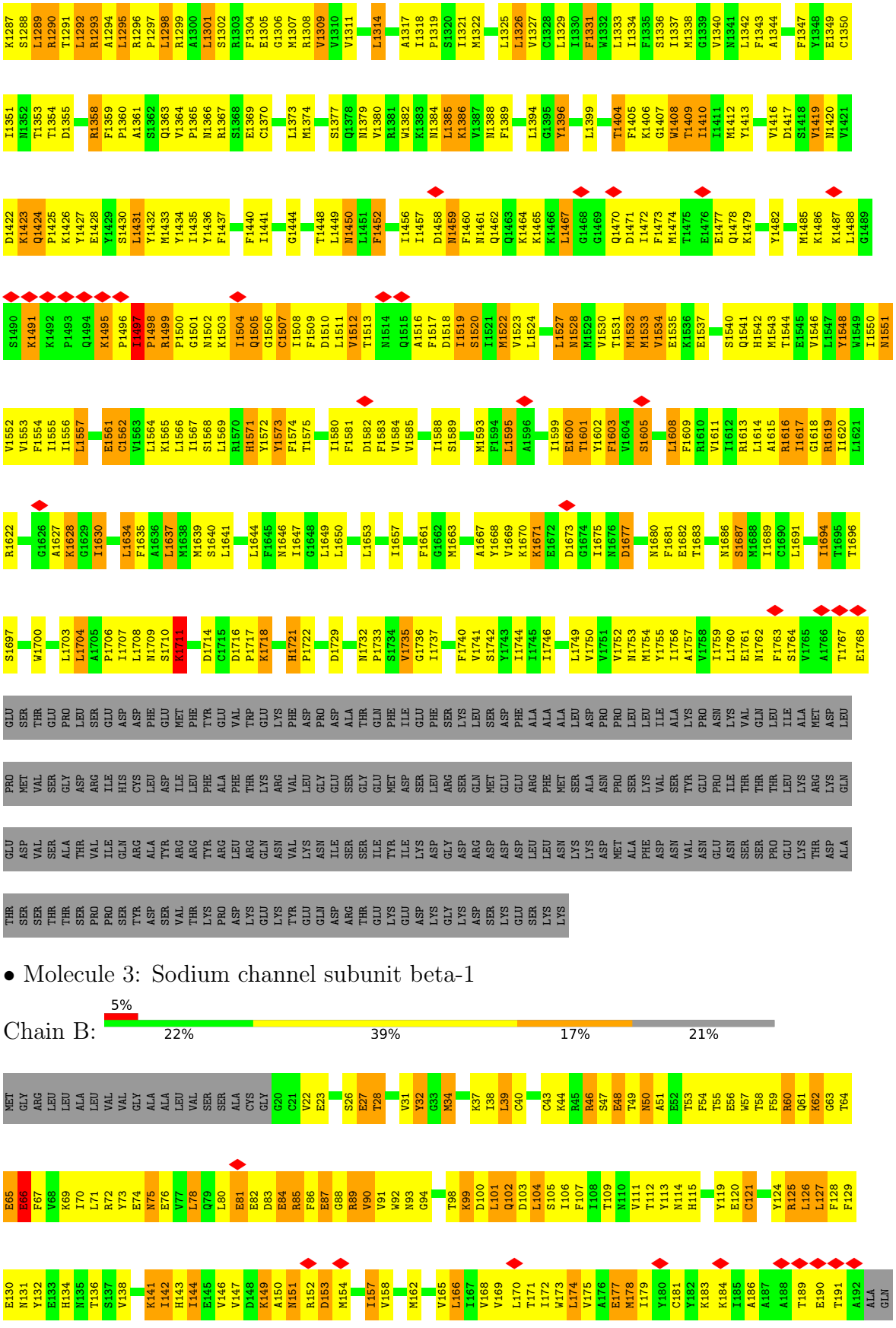
• Molecule 1: Sodium channel subunit beta-2



• Molecule 2: Sodium channel protein type 9 subunit alpha





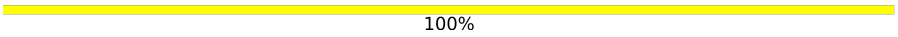


• Molecule 3: Sodium channel subunit beta-1

Chain B:

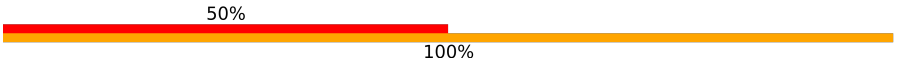
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	263205	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 ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.349	Depositor
Minimum map value	-0.210	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	261.84, 261.84, 261.84	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.091, 1.091, 1.091	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, 9SR

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	C	0.50	1/1002 (0.1%)	0.66	1/1354 (0.1%)
2	A	0.50	0/9417	0.65	4/12761 (0.0%)
3	B	0.44	0/1442	0.64	0/1949
All	All	0.49	1/11861 (0.0%)	0.65	5/16064 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	127	CYS	CB-SG	11.15	2.01	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1497	ILE	C-N-CD	-8.47	101.96	120.60
1	C	127	CYS	CA-CB-SG	7.89	128.21	114.00
2	A	925	CYS	N-CA-C	-6.18	94.30	111.00
2	A	228	ILE	C-N-CD	5.02	138.94	128.40
2	A	1721	HIS	C-N-CD	5.00	138.90	128.40

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	C	980	0	942	138	0
2	A	9192	0	9420	1287	0
3	B	1416	0	1378	220	0
4	D	28	0	25	0	0
4	E	28	0	25	7	0
5	A	28	0	26	1	0
5	B	56	0	52	1	0
5	C	14	0	13	15	0
6	A	22	0	0	1	0
All	All	11764	0	11881	1625	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 69.

All (1625) 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)
2:A:1497:ILE:HG23	2:A:1572:TYR:CD2	1.39	1.53
2:A:794:LYS:HB3	2:A:803:TYR:CE2	1.50	1.44
2:A:851:THR:CG2	2:A:1327:VAL:HG21	1.43	1.44
2:A:1500:PRO:CG	2:A:1505:GLN:HB3	1.45	1.42
2:A:735:LYS:NZ	2:A:739:PHE:HB2	1.27	1.41
1:C:82:GLN:NE2	5:C:301:NAG:H82	1.30	1.40
2:A:855:LEU:HD21	2:A:1331:PHE:CD2	1.56	1.39
2:A:251:LEU:HD13	2:A:1630:ILE:CG2	1.52	1.39
2:A:174:ARG:HD3	2:A:182:THR:CG2	1.55	1.37
2:A:1295:LEU:CD1	2:A:1298:LEU:HD23	1.54	1.35
3:B:67:PHE:CE2	3:B:120:GLU:HG3	1.59	1.34
2:A:1497:ILE:CG2	2:A:1572:TYR:CD2	2.09	1.33
2:A:1668:TYR:CD1	2:A:1721:HIS:CE1	2.16	1.33
2:A:855:LEU:HD21	2:A:1331:PHE:CE2	1.60	1.32
2:A:221:ALA:O	2:A:224:THR:HG23	1.24	1.32
2:A:1238:ILE:CD1	2:A:1270:LEU:HD23	1.59	1.32
1:C:65:LEU:CD1	1:C:110:VAL:HB	1.58	1.32
2:A:1295:LEU:CD1	2:A:1298:LEU:CD2	2.11	1.28
2:A:157:TYR:O	2:A:160:THR:HG22	1.29	1.25
2:A:855:LEU:CD2	2:A:1331:PHE:CD2	2.18	1.25
3:B:51:ALA:CB	3:B:127:LEU:HD12	1.66	1.24
2:A:179:GLY:O	2:A:180:GLU:HG2	1.31	1.24
2:A:1496:PRO:O	2:A:1497:ILE:HD12	1.29	1.24
1:C:82:GLN:CD	5:C:301:NAG:H82	1.57	1.23
2:A:1238:ILE:HD11	2:A:1270:LEU:CD2	1.69	1.23

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:171:ILE:HG22	2:A:183:PHE:CE2	1.72	1.22
2:A:839:LEU:HD11	2:A:1337:ILE:CG2	1.68	1.22
1:C:128:TYR:CD2	1:C:137:ARG:NH2	2.09	1.21
2:A:839:LEU:CD1	2:A:1337:ILE:HG21	1.71	1.21
2:A:1532:MET:CE	2:A:1620:ILE:HD11	1.69	1.20
2:A:251:LEU:CD1	2:A:1630:ILE:HG22	1.69	1.20
2:A:336:ASN:ND2	2:A:343:SER:HB3	1.55	1.20
3:B:51:ALA:HB2	3:B:127:LEU:CD1	1.72	1.20
2:A:794:LYS:CB	2:A:803:TYR:HE2	1.53	1.19
2:A:811:PHE:CE1	2:A:815:ILE:HD11	1.79	1.18
1:C:82:GLN:NE2	5:C:301:NAG:C8	2.07	1.17
2:A:855:LEU:CD2	2:A:1331:PHE:CE2	2.27	1.17
2:A:174:ARG:HD3	2:A:182:THR:HG21	1.25	1.17
2:A:1430:SER:OG	2:A:1433:MET:HG2	1.42	1.17
1:C:128:TYR:CD2	1:C:137:ARG:CZ	2.27	1.17
3:B:67:PHE:HE2	3:B:120:GLU:CG	1.58	1.17
2:A:1546:VAL:O	2:A:1550:ILE:HG13	1.46	1.16
2:A:735:LYS:NZ	2:A:739:PHE:CB	2.09	1.16
3:B:71:LEU:CB	3:B:80:LEU:HD12	1.76	1.15
2:A:839:LEU:CD1	2:A:1337:ILE:CG2	2.25	1.14
2:A:1532:MET:HE3	2:A:1620:ILE:HD11	1.21	1.13
2:A:1694:ILE:CD1	2:A:1703:LEU:HD12	1.78	1.13
3:B:71:LEU:HB2	3:B:80:LEU:HD12	1.20	1.13
2:A:251:LEU:CD1	2:A:1630:ILE:CG2	2.26	1.12
2:A:174:ARG:HB3	2:A:182:THR:HB	1.30	1.11
2:A:1647:ILE:CG2	2:A:1754:MET:CE	2.29	1.11
2:A:149:PRO:O	2:A:152:THR:HG22	1.49	1.10
2:A:851:THR:HG22	2:A:1327:VAL:HG21	1.20	1.10
2:A:1500:PRO:CG	2:A:1505:GLN:CB	2.27	1.10
2:A:743:ASP:OD1	2:A:744:PRO:HD3	1.47	1.10
2:A:171:ILE:HG22	2:A:183:PHE:CD2	1.85	1.10
2:A:1647:ILE:HG21	2:A:1754:MET:HE2	1.19	1.10
2:A:1694:ILE:HD11	2:A:1703:LEU:HD12	1.31	1.09
2:A:136:ILE:HD11	2:A:224:THR:HG22	1.31	1.09
2:A:960:LEU:CD2	2:A:964:LEU:HD23	1.82	1.09
2:A:1295:LEU:HD12	2:A:1298:LEU:HD23	1.18	1.09
2:A:742:MET:C	2:A:744:PRO:HD2	1.71	1.08
2:A:1647:ILE:HG21	2:A:1754:MET:CE	1.84	1.08
2:A:960:LEU:HD23	2:A:964:LEU:HD23	1.34	1.07
2:A:823:LEU:HD12	2:A:824:PHE:HD1	1.18	1.07
3:B:91:VAL:HG23	3:B:107:PHE:HB3	1.33	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:851:THR:HG21	2:A:1327:VAL:HG21	1.16	1.07
2:A:899:ILE:O	2:A:900:ASN:ND2	1.88	1.07
2:A:1457:ILE:HG22	2:A:1756:ILE:HD11	1.36	1.07
2:A:1485:MET:HB3	2:A:1639:MET:HE3	1.37	1.06
1:C:63:PHE:HE2	1:C:105:PRO:HB3	1.21	1.06
2:A:1668:TYR:CB	2:A:1721:HIS:HE1	1.68	1.06
2:A:174:ARG:CD	2:A:182:THR:HG22	1.83	1.06
1:C:107:LYS:HZ2	1:C:109:ASP:CB	1.69	1.05
2:A:1764:SER:O	2:A:1767:THR:HG22	1.56	1.05
2:A:1298:LEU:HD12	2:A:1301:LEU:HD12	1.36	1.05
1:C:107:LYS:NZ	1:C:109:ASP:CB	2.20	1.05
3:B:92:TRP:CE2	3:B:94:GLY:HA3	1.92	1.05
2:A:293:LEU:HD12	2:A:298:ASP:CB	1.87	1.04
2:A:735:LYS:HZ1	2:A:739:PHE:CB	1.69	1.04
1:C:101:PHE:CE2	1:C:103:GLY:O	2.11	1.04
2:A:798:MET:O	2:A:802:GLU:HB2	1.55	1.04
2:A:174:ARG:CD	2:A:182:THR:CG2	2.33	1.04
2:A:851:THR:CG2	2:A:1327:VAL:CG2	2.34	1.04
2:A:1251:LYS:O	2:A:1255:THR:HG23	1.58	1.04
2:A:1295:LEU:HD11	2:A:1298:LEU:CD2	1.88	1.04
3:B:54:PHE:CZ	3:B:124:TYR:HD2	1.76	1.04
2:A:1500:PRO:HG3	2:A:1505:GLN:CG	1.88	1.03
2:A:1668:TYR:CG	2:A:1721:HIS:HE1	1.76	1.03
2:A:136:ILE:CD1	2:A:224:THR:HG22	1.88	1.03
2:A:849:TRP:HD1	2:A:850:PRO:HD2	1.20	1.03
2:A:1541:GLN:OE1	2:A:1541:GLN:N	1.89	1.03
2:A:136:ILE:HD11	2:A:224:THR:CG2	1.88	1.03
2:A:840:LEU:HD12	2:A:843:PHE:HE2	1.23	1.02
2:A:1353:THR:HG23	2:A:1379:ASN:O	1.59	1.02
2:A:132:ILE:HD11	2:A:166:GLU:HB3	1.38	1.02
2:A:795:LEU:HD23	2:A:803:TYR:CE2	1.95	1.02
2:A:1668:TYR:CD1	2:A:1721:HIS:ND1	2.25	1.02
2:A:896:VAL:HG23	2:A:897:CYS:H	1.21	1.02
2:A:1457:ILE:HG22	2:A:1756:ILE:CD1	1.90	1.01
2:A:862:SER:O	2:A:870:THR:HG21	1.60	1.01
2:A:1668:TYR:HB3	2:A:1721:HIS:HE1	1.25	1.01
1:C:65:LEU:HD11	1:C:110:VAL:HB	1.38	1.00
2:A:293:LEU:HD12	2:A:298:ASP:HB3	1.01	1.00
2:A:899:ILE:HG21	2:A:934:ASP:OD2	1.62	1.00
2:A:1218:ARG:O	2:A:1219:LYS:HG2	1.61	1.00
2:A:1295:LEU:HD11	2:A:1298:LEU:HD23	1.42	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:823:LEU:HD12	2:A:824:PHE:CD1	1.96	1.00
3:B:39:LEU:HD23	3:B:105:SER:OG	1.60	1.00
3:B:51:ALA:CB	3:B:127:LEU:CD1	2.32	1.00
1:C:65:LEU:CD1	1:C:110:VAL:CB	2.39	1.00
2:A:154:ASN:HA	2:A:157:TYR:HD2	1.25	0.99
2:A:336:ASN:ND2	2:A:343:SER:CB	2.26	0.99
2:A:851:THR:HG21	2:A:1327:VAL:CG2	1.91	0.99
2:A:839:LEU:HD11	2:A:1337:ILE:HG22	1.41	0.99
2:A:1668:TYR:HD1	2:A:1721:HIS:CE1	1.74	0.99
3:B:91:VAL:CG2	3:B:107:PHE:HB3	1.92	0.99
2:A:735:LYS:HZ1	2:A:739:PHE:HB2	1.16	0.98
2:A:791:MET:O	2:A:795:LEU:HD21	1.61	0.98
1:C:62:GLN:O	1:C:132:PRO:CD	2.11	0.98
2:A:844:LYS:O	2:A:847:LYS:CE	2.11	0.98
2:A:847:LYS:H	2:A:847:LYS:HD2	1.28	0.98
2:A:855:LEU:CD2	2:A:1331:PHE:HD2	1.67	0.98
3:B:92:TRP:CZ2	3:B:94:GLY:HA3	1.96	0.98
2:A:1496:PRO:O	2:A:1497:ILE:CD1	2.12	0.98
3:B:54:PHE:CZ	3:B:124:TYR:CD2	2.50	0.98
3:B:34:MET:O	3:B:111:VAL:HG23	1.64	0.98
2:A:1595:LEU:O	2:A:1599:ILE:HD12	1.64	0.97
2:A:1504:ILE:HD13	2:A:1505:GLN:H	1.28	0.97
2:A:1430:SER:OG	2:A:1433:MET:CG	2.12	0.97
2:A:1374:MET:HG2	2:A:1380:VAL:HG13	1.46	0.97
3:B:71:LEU:CB	3:B:80:LEU:CD1	2.43	0.97
1:C:128:TYR:HD2	1:C:137:ARG:CZ	1.74	0.97
2:A:1500:PRO:HG2	2:A:1505:GLN:CB	1.91	0.97
2:A:1677:ASP:OD1	2:A:1677:ASP:O	1.83	0.96
2:A:293:LEU:CD1	2:A:298:ASP:HB3	1.95	0.96
2:A:733:PHE:CE1	2:A:796:ILE:HG21	2.00	0.96
2:A:1627:ALA:HB3	2:A:1630:ILE:CD1	1.96	0.96
2:A:735:LYS:HZ3	2:A:739:PHE:HB2	1.25	0.96
1:C:52:PHE:O	1:C:108:TYR:HB3	1.63	0.96
2:A:1668:TYR:HB3	2:A:1721:HIS:CE1	2.01	0.95
2:A:1532:MET:CE	2:A:1620:ILE:CD1	2.44	0.95
2:A:221:ALA:O	2:A:224:THR:CG2	2.14	0.95
3:B:171:THR:O	3:B:175:VAL:HG23	1.66	0.95
2:A:305:TYR:HE1	2:A:311:ASP:HA	1.29	0.95
1:C:107:LYS:HZ2	1:C:109:ASP:HB3	1.28	0.95
2:A:1716:ASP:OD1	2:A:1717:PRO:HD2	1.66	0.94
2:A:928:TRP:CD1	2:A:952:MET:SD	2.60	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1497:ILE:CG2	2:A:1572:TYR:HD2	1.65	0.94
3:B:71:LEU:HB2	3:B:80:LEU:CD1	1.95	0.94
2:A:1755:TYR:O	2:A:1759:ILE:HG12	1.67	0.94
2:A:1500:PRO:HG2	2:A:1505:GLN:HB3	0.95	0.94
2:A:1238:ILE:CD1	2:A:1270:LEU:CD2	2.36	0.94
2:A:1668:TYR:CG	2:A:1721:HIS:CE1	2.54	0.94
2:A:132:ILE:HD11	2:A:166:GLU:CB	1.96	0.94
2:A:213:LEU:HD23	2:A:214:ARG:N	1.83	0.94
2:A:226:SER:HA	2:A:232:LYS:HE3	1.48	0.94
2:A:171:ILE:CG2	2:A:183:PHE:CE2	2.51	0.94
2:A:148:PRO:HB2	2:A:152:THR:HG21	1.49	0.93
2:A:399:ALA:CB	2:A:1762:ASN:HD22	1.82	0.93
2:A:839:LEU:HD12	2:A:1337:ILE:HG21	1.47	0.93
2:A:1213:ASP:HB3	2:A:1663:MET:CE	1.97	0.93
2:A:1353:THR:OG1	2:A:1379:ASN:HB3	1.68	0.93
2:A:839:LEU:HD11	2:A:1337:ILE:HG21	1.36	0.93
2:A:188:TRP:CD1	2:A:232:LYS:HE2	2.04	0.93
2:A:1532:MET:HE3	2:A:1620:ILE:CD1	1.99	0.93
3:B:26:SER:OG	3:B:142:ILE:HG21	1.69	0.93
3:B:92:TRP:NE1	3:B:94:GLY:CA	2.32	0.93
2:A:213:LEU:HD23	2:A:214:ARG:HG2	1.51	0.93
2:A:733:PHE:CZ	2:A:737:ILE:HG21	2.04	0.92
2:A:1350:CYS:SG	2:A:1382:TRP:HE3	1.92	0.92
2:A:755:VAL:O	2:A:758:THR:HG22	1.69	0.92
3:B:87:GLU:OE2	3:B:88:GLY:N	2.01	0.92
2:A:1647:ILE:CG2	2:A:1754:MET:HE2	1.95	0.92
2:A:1506:GLY:O	2:A:1510:ASP:CG	2.07	0.92
2:A:1512:VAL:HG12	2:A:1517:PHE:HE2	1.33	0.92
2:A:207:LEU:HG	2:A:209:ASN:OD1	1.68	0.92
2:A:735:LYS:NZ	2:A:735:LYS:O	2.02	0.92
2:A:213:LEU:CD2	2:A:214:ARG:HG2	1.99	0.91
2:A:399:ALA:CB	2:A:1762:ASN:ND2	2.33	0.91
3:B:67:PHE:CE2	3:B:120:GLU:CG	2.39	0.91
1:C:52:PHE:HB2	1:C:129:ILE:HD13	1.50	0.91
1:C:62:GLN:O	1:C:132:PRO:HD3	1.71	0.91
1:C:82:GLN:HE22	5:C:301:NAG:H82	1.21	0.91
2:A:967:LEU:CD2	2:A:968:LEU:HD13	2.01	0.91
2:A:1295:LEU:CD1	2:A:1298:LEU:HD22	2.01	0.91
2:A:157:TYR:O	2:A:160:THR:CG2	2.18	0.91
2:A:743:ASP:OD1	2:A:744:PRO:CD	2.18	0.91
1:C:135:ARG:HG2	1:C:135:ARG:HH21	1.36	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1512:VAL:HG12	2:A:1517:PHE:CE2	2.06	0.90
2:A:1432:TYR:O	2:A:1435:ILE:HG12	1.71	0.90
2:A:1627:ALA:HB3	2:A:1630:ILE:HD12	1.53	0.90
2:A:1288:SER:O	2:A:1291:THR:HG22	1.70	0.90
2:A:855:LEU:HD21	2:A:1331:PHE:HE2	1.36	0.89
2:A:1274:VAL:HA	2:A:1277:THR:HG22	1.54	0.89
1:C:82:GLN:NE2	5:C:301:NAG:C7	2.35	0.89
2:A:117:ARG:HB3	2:A:117:ARG:HH11	1.35	0.89
2:A:849:TRP:CD1	2:A:850:PRO:HD2	2.07	0.89
2:A:167:SER:O	2:A:171:ILE:HG23	1.71	0.89
2:A:399:ALA:HB1	2:A:1762:ASN:ND2	1.88	0.89
2:A:1502:ASN:HB3	2:A:1504:ILE:CD1	2.03	0.88
1:C:59:ASN:CB	1:C:62:GLN:HB2	2.03	0.88
2:A:791:MET:HG3	2:A:816:VAL:HG21	1.53	0.88
2:A:851:THR:HG22	2:A:1327:VAL:CG2	2.01	0.88
2:A:936:MET:CE	2:A:945:LEU:HG	2.02	0.88
2:A:1497:ILE:HG23	2:A:1572:TYR:CE2	2.06	0.88
2:A:855:LEU:HD21	2:A:1331:PHE:HD2	1.28	0.88
1:C:63:PHE:HE1	1:C:129:ILE:CG2	1.86	0.88
2:A:168:LEU:HD23	2:A:169:VAL:N	1.87	0.88
2:A:196:ILE:HD12	2:A:197:VAL:HG23	1.56	0.88
2:A:321:SER:HB3	2:A:375:GLY:HA2	1.55	0.88
1:C:34:VAL:HG12	1:C:50:CYS:SG	2.13	0.87
2:A:1581:PHE:O	2:A:1585:VAL:HG13	1.73	0.87
1:C:52:PHE:CB	1:C:129:ILE:HD13	2.03	0.87
3:B:55:THR:OG1	3:B:104:LEU:CD2	2.23	0.87
2:A:174:ARG:HD2	2:A:182:THR:HG22	1.56	0.87
2:A:772:PHE:CE1	2:A:776:LEU:HD21	2.09	0.87
1:C:63:PHE:HE1	1:C:129:ILE:HG22	1.39	0.87
2:A:817:THR:O	2:A:821:VAL:HG23	1.75	0.87
2:A:1293:ARG:HB3	2:A:1293:ARG:HH21	1.39	0.87
2:A:164:THR:HG21	2:A:200:TYR:OH	1.75	0.86
2:A:117:ARG:HH11	2:A:117:ARG:CB	1.87	0.86
2:A:179:GLY:O	2:A:180:GLU:CG	2.22	0.86
2:A:807:GLY:O	2:A:810:ILE:CG1	2.23	0.86
2:A:1639:MET:CE	2:A:1639:MET:HA	2.04	0.86
2:A:1532:MET:HE1	2:A:1620:ILE:HD11	1.56	0.86
2:A:928:TRP:CZ3	2:A:929:ILE:HD12	2.10	0.86
2:A:835:ARG:O	2:A:838:ARG:HG3	1.75	0.86
2:A:1647:ILE:HG22	2:A:1754:MET:CE	2.04	0.86
2:A:367:TYR:OH	2:A:1689:ILE:HG23	1.76	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1452:PHE:O	2:A:1456:ILE:HD12	1.75	0.86
2:A:1668:TYR:O	2:A:1729:ASP:CB	2.24	0.86
2:A:1186:TYR:O	2:A:1190:GLU:HG2	1.75	0.85
2:A:840:LEU:HD12	2:A:843:PHE:CE2	2.11	0.85
2:A:1298:LEU:HD12	2:A:1301:LEU:CD1	2.07	0.85
1:C:69:TYR:HE2	1:C:94:ARG:NH1	1.75	0.85
2:A:772:PHE:O	2:A:776:LEU:HD23	1.77	0.85
1:C:66:ASN:ND2	1:C:79:MET:CE	2.40	0.85
2:A:733:PHE:HE1	2:A:796:ILE:HG21	1.40	0.85
2:A:1384:ASN:OD1	2:A:1388:ASN:ND2	2.09	0.85
2:A:1499:ARG:HH11	2:A:1501:GLY:HA2	1.42	0.85
2:A:1293:ARG:HH21	2:A:1293:ARG:CB	1.90	0.84
2:A:1500:PRO:HG3	2:A:1505:GLN:CB	2.02	0.84
2:A:1582:ASP:O	2:A:1585:VAL:HG22	1.76	0.84
1:C:63:PHE:CE2	1:C:105:PRO:HB3	2.10	0.84
2:A:855:LEU:HD23	2:A:1331:PHE:CD2	2.10	0.84
2:A:1229:ALA:O	2:A:1232:ILE:HG22	1.76	0.84
2:A:1457:ILE:HD12	2:A:1458:ASP:N	1.92	0.84
3:B:86:PHE:HZ	3:B:119:TYR:HH	0.87	0.84
3:B:71:LEU:HB3	3:B:80:LEU:CD1	2.07	0.84
1:C:65:LEU:HD12	1:C:110:VAL:CB	2.08	0.84
3:B:28:THR:HG22	3:B:143:HIS:O	1.78	0.84
2:A:286:LEU:HD11	2:A:333:ILE:HG13	1.59	0.83
2:A:795:LEU:O	2:A:799:ASP:N	2.11	0.83
1:C:33:THR:O	1:C:50:CYS:HA	1.79	0.83
2:A:795:LEU:HD23	2:A:795:LEU:H	1.42	0.83
2:A:795:LEU:CD2	2:A:803:TYR:CE2	2.61	0.83
2:A:928:TRP:HZ3	2:A:929:ILE:HD12	1.42	0.83
2:A:1350:CYS:SG	2:A:1382:TRP:CE3	2.70	0.83
2:A:284:GLU:OE1	2:A:289:ILE:HD11	1.78	0.83
2:A:153:LYS:CE	2:A:157:TYR:OH	2.26	0.83
2:A:275:CYS:SG	2:A:324:CYS:HB3	2.19	0.83
2:A:1497:ILE:HG23	2:A:1572:TYR:CG	2.14	0.83
2:A:153:LYS:HE3	2:A:157:TYR:OH	1.79	0.83
3:B:46:ARG:HD3	3:B:48:GLU:OE2	1.78	0.83
1:C:32:VAL:CG1	1:C:50:CYS:SG	2.67	0.83
2:A:196:ILE:CD1	2:A:197:VAL:HG23	2.09	0.83
2:A:1616:ARG:O	2:A:1618:GLY:N	2.12	0.83
2:A:179:GLY:C	2:A:180:GLU:HG2	2.00	0.82
2:A:794:LYS:CB	2:A:803:TYR:CE2	2.41	0.82
2:A:119:SER:O	2:A:122:ILE:HG22	1.79	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:795:LEU:HD23	2:A:795:LEU:N	1.95	0.82
3:B:55:THR:OG1	3:B:104:LEU:HD23	1.79	0.82
1:C:79:MET:HE1	5:C:301:NAG:C1	2.10	0.82
2:A:869:LEU:HD12	2:A:869:LEU:O	1.78	0.82
3:B:72:ARG:HH22	3:B:74:GLU:CD	1.81	0.82
1:C:82:GLN:CD	5:C:301:NAG:C8	2.40	0.82
3:B:34:MET:O	3:B:111:VAL:CG2	2.26	0.82
2:A:1213:ASP:HB3	2:A:1663:MET:HE3	1.62	0.82
2:A:1283:LEU:HD23	2:A:1283:LEU:H	1.45	0.82
2:A:1574:PHE:HD1	2:A:1580:ILE:HD11	1.45	0.82
2:A:1532:MET:HE1	2:A:1620:ILE:CD1	2.10	0.82
3:B:54:PHE:CE1	3:B:124:TYR:HD2	1.97	0.82
2:A:199:ALA:O	2:A:202:THR:HG22	1.79	0.82
2:A:1509:PHE:HB2	2:A:1568:SER:HB3	1.61	0.81
2:A:1546:VAL:O	2:A:1550:ILE:CG1	2.26	0.81
2:A:852:LEU:O	2:A:856:ILE:HG12	1.80	0.81
3:B:51:ALA:HB2	3:B:127:LEU:HD12	0.84	0.81
2:A:305:TYR:HE1	2:A:311:ASP:CA	1.93	0.81
2:A:741:VAL:O	2:A:746:VAL:CG2	2.28	0.81
2:A:936:MET:HE1	2:A:945:LEU:CD1	2.10	0.81
3:B:86:PHE:HZ	3:B:119:TYR:OH	1.62	0.81
2:A:736:CYS:O	2:A:740:ILE:HG12	1.80	0.81
2:A:737:ILE:HD11	2:A:797:ALA:CA	2.11	0.81
2:A:327:GLY:O	3:B:132:TYR:HE2	1.61	0.81
2:A:849:TRP:HD1	2:A:850:PRO:CD	1.92	0.81
2:A:1268:VAL:HG13	2:A:1289:LEU:HD13	1.62	0.81
3:B:39:LEU:CD2	3:B:105:SER:OG	2.29	0.81
4:E:1:NAG:H3	4:E:1:NAG:H83	1.61	0.81
2:A:742:MET:C	2:A:744:PRO:CD	2.49	0.81
2:A:811:PHE:HE1	2:A:815:ILE:HD11	1.43	0.81
1:C:65:LEU:HD12	1:C:110:VAL:HB	1.60	0.81
2:A:249:MET:O	2:A:253:VAL:HG23	1.81	0.80
3:B:103:ASP:C	3:B:104:LEU:HD12	2.02	0.80
2:A:188:TRP:NE1	2:A:232:LYS:HE2	1.95	0.80
2:A:1485:MET:HB3	2:A:1639:MET:CE	2.11	0.80
2:A:1639:MET:HA	2:A:1639:MET:HE2	1.64	0.80
2:A:412:ASN:O	2:A:415:GLU:HG3	1.82	0.80
2:A:737:ILE:HD11	2:A:797:ALA:HA	1.62	0.80
1:C:107:LYS:NZ	1:C:109:ASP:CG	2.34	0.80
1:C:128:TYR:CG	1:C:137:ARG:NH2	2.49	0.80
2:A:410:GLN:O	2:A:413:ILE:HG22	1.80	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:141:LYS:HZ2	3:B:141:LYS:HB3	1.47	0.80
2:A:737:ILE:HG13	2:A:738:TYR:N	1.96	0.80
3:B:67:PHE:HE2	3:B:120:GLU:HG3	0.71	0.80
4:E:2:NAG:O7	4:E:2:NAG:O3	1.98	0.80
3:B:89:ARG:HG3	3:B:89:ARG:HH11	1.47	0.80
1:C:33:THR:O	1:C:51:THR:N	2.15	0.79
1:C:47:ARG:O	1:C:49:PRO:HD3	1.81	0.79
2:A:116:ARG:HH12	2:A:176:PHE:CB	1.95	0.79
2:A:807:GLY:O	2:A:810:ILE:HG13	1.83	0.79
2:A:163:TYR:HE2	2:A:220:ARG:HG2	1.47	0.79
2:A:791:MET:O	2:A:795:LEU:CD2	2.30	0.79
2:A:1616:ARG:HG3	2:A:1616:ARG:HH11	1.46	0.79
2:A:226:SER:CA	2:A:232:LYS:HE3	2.13	0.79
1:C:66:ASN:ND2	1:C:79:MET:HE2	1.97	0.79
2:A:824:PHE:C	2:A:825:LEU:HD12	2.03	0.79
2:A:1270:LEU:HD13	2:A:1270:LEU:O	1.83	0.79
2:A:251:LEU:HD13	2:A:1630:ILE:HG22	0.80	0.78
2:A:895:CYS:CB	2:A:938:VAL:HG12	2.13	0.78
1:C:59:ASN:HB2	1:C:62:GLN:HB2	1.65	0.78
1:C:107:LYS:NZ	1:C:109:ASP:HB2	1.95	0.78
2:A:879:ILE:O	2:A:883:VAL:HG23	1.84	0.78
2:A:184:LEU:CD1	2:A:190:TRP:CD1	2.66	0.78
2:A:305:TYR:CE1	2:A:312:ALA:N	2.52	0.78
2:A:1295:LEU:HD13	2:A:1298:LEU:HD22	1.65	0.78
3:B:92:TRP:NE1	3:B:94:GLY:N	2.31	0.78
2:A:733:PHE:CZ	2:A:737:ILE:CG2	2.66	0.78
2:A:1732:ASN:OD1	2:A:1735:VAL:HB	1.84	0.77
2:A:1410:ILE:HD12	2:A:1410:ILE:O	1.83	0.77
2:A:1709:ASN:HB2	2:A:1714:ASP:HB3	1.67	0.77
2:A:164:THR:CG2	2:A:200:TYR:OH	2.32	0.77
2:A:1588:ILE:HG22	2:A:1615:ALA:HB1	1.64	0.77
1:C:62:GLN:O	1:C:132:PRO:HD2	1.85	0.77
2:A:733:PHE:HE1	2:A:796:ILE:CG2	1.97	0.77
2:A:1218:ARG:O	2:A:1219:LYS:CG	2.32	0.77
2:A:131:LEU:HD22	2:A:131:LEU:O	1.84	0.77
1:C:59:ASN:HB3	1:C:62:GLN:HB2	1.67	0.77
2:A:733:PHE:CE1	2:A:737:ILE:HG21	2.20	0.77
4:E:1:NAG:H3	4:E:1:NAG:C8	2.14	0.77
1:C:33:THR:HB	1:C:51:THR:CB	2.14	0.77
2:A:305:TYR:CE1	2:A:311:ASP:C	2.58	0.77
3:B:51:ALA:HB1	3:B:126:LEU:O	1.85	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:282:ASN:O	5:A:2006:NAG:H82	1.84	0.76
2:A:336:ASN:CG	2:A:343:SER:OG	2.24	0.76
2:A:795:LEU:CD2	2:A:803:TYR:CZ	2.69	0.76
1:C:32:VAL:HA	1:C:51:THR:O	1.85	0.76
1:C:52:PHE:HB2	1:C:129:ILE:CD1	2.15	0.76
1:C:69:TYR:CE2	1:C:94:ARG:NH1	2.52	0.76
1:C:79:MET:CE	5:C:301:NAG:C1	2.64	0.76
2:A:895:CYS:O	2:A:897:CYS:N	2.17	0.76
2:A:184:LEU:HD11	2:A:190:TRP:HD1	1.50	0.76
2:A:361:ASP:OD2	2:A:929:ILE:HG22	1.84	0.76
2:A:207:LEU:HD21	2:A:209:ASN:HD21	1.48	0.76
2:A:1374:MET:CG	2:A:1380:VAL:HG13	2.15	0.76
3:B:71:LEU:HD21	3:B:106:ILE:HD12	1.68	0.76
2:A:116:ARG:HH12	2:A:176:PHE:HB2	1.48	0.76
2:A:849:TRP:CE3	2:A:852:LEU:HD22	2.21	0.76
2:A:1512:VAL:HA	2:A:1517:PHE:CD2	2.21	0.76
2:A:795:LEU:HD22	2:A:803:TYR:CZ	2.21	0.76
2:A:1502:ASN:CB	2:A:1504:ILE:CD1	2.65	0.76
1:C:107:LYS:HD2	1:C:109:ASP:HB2	1.67	0.75
1:C:107:LYS:HZ3	1:C:109:ASP:CB	1.98	0.75
3:B:58:THR:HG22	3:B:69:LYS:HA	1.67	0.75
2:A:839:LEU:HD12	2:A:1337:ILE:CG2	2.08	0.75
2:A:1268:VAL:CG1	2:A:1289:LEU:HD13	2.15	0.75
2:A:1500:PRO:CG	2:A:1505:GLN:CG	2.60	0.75
3:B:165:VAL:O	3:B:169:VAL:HG23	1.87	0.75
2:A:240:GLN:OE1	2:A:240:GLN:HA	1.85	0.75
2:A:1627:ALA:CB	2:A:1630:ILE:HD11	2.16	0.75
2:A:928:TRP:NE1	2:A:952:MET:SD	2.60	0.75
2:A:327:GLY:HA3	3:B:134:HIS:CD2	2.21	0.75
2:A:1274:VAL:O	2:A:1278:LEU:N	2.18	0.75
3:B:174:LEU:HD13	3:B:174:LEU:O	1.86	0.75
2:A:196:ILE:HD12	2:A:197:VAL:CG2	2.16	0.75
2:A:407:GLU:HG3	2:A:408:GLN:N	2.02	0.75
1:C:103:GLY:O	1:C:105:PRO:HD3	1.87	0.75
2:A:207:LEU:HD12	2:A:208:GLY:H	1.50	0.75
2:A:1499:ARG:HH11	2:A:1501:GLY:CA	1.99	0.74
3:B:72:ARG:NH2	3:B:74:GLU:OE2	2.20	0.74
2:A:154:ASN:HA	2:A:157:TYR:CD2	2.15	0.74
2:A:1627:ALA:CB	2:A:1630:ILE:CD1	2.65	0.74
3:B:92:TRP:CE2	3:B:94:GLY:CA	2.67	0.74
2:A:752:ILE:O	2:A:755:VAL:HG12	1.87	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:GLN:OE1	5:C:301:NAG:H82	1.85	0.74
2:A:844:LYS:O	2:A:847:LYS:CD	2.35	0.74
2:A:909:HIS:HD2	2:A:911:ASN:H	1.34	0.74
2:A:1497:ILE:HG21	2:A:1572:TYR:HD2	1.53	0.74
2:A:813:SER:HA	2:A:816:VAL:HG23	1.69	0.74
2:A:839:LEU:CD1	2:A:1337:ILE:HG22	2.06	0.74
2:A:971:PHE:CE2	2:A:1458:ASP:OD2	2.40	0.74
2:A:1553:VAL:HG12	2:A:1557:LEU:HD22	1.70	0.74
1:C:107:LYS:HZ3	1:C:109:ASP:CG	1.89	0.74
2:A:219:LEU:HD22	2:A:222:LEU:HD13	1.69	0.74
3:B:126:LEU:HD13	3:B:128:PHE:CZ	2.22	0.74
1:C:63:PHE:CE1	1:C:129:ILE:CG2	2.70	0.74
2:A:737:ILE:O	2:A:740:ILE:N	2.21	0.74
2:A:366:LEU:O	2:A:370:THR:HG23	1.88	0.74
1:C:101:PHE:HE2	1:C:103:GLY:O	1.69	0.73
2:A:118:ILE:HD13	2:A:118:ILE:N	2.03	0.73
2:A:278:ASN:ND2	2:A:329:THR:OG1	2.21	0.73
2:A:896:VAL:HG23	2:A:897:CYS:N	2.00	0.73
2:A:1668:TYR:CB	2:A:1721:HIS:CE1	2.60	0.73
2:A:184:LEU:HD11	2:A:190:TRP:CD1	2.23	0.73
2:A:960:LEU:HD21	2:A:964:LEU:HD23	1.68	0.73
1:C:58:VAL:HG13	1:C:63:PHE:HB2	1.69	0.73
2:A:1616:ARG:HG3	2:A:1616:ARG:NH1	2.01	0.73
2:A:1294:ALA:O	2:A:1297:PRO:HD2	1.89	0.73
2:A:1750:VAL:O	2:A:1753:ASN:HB2	1.88	0.73
2:A:116:ARG:HH12	2:A:176:PHE:CA	2.00	0.73
2:A:245:LEU:HD13	2:A:249:MET:CE	2.19	0.73
2:A:1535:GLU:OE2	2:A:1613:ARG:NH1	2.22	0.73
3:B:168:VAL:O	3:B:172:ILE:HG13	1.86	0.73
1:C:65:LEU:HD13	1:C:110:VAL:HB	1.67	0.73
2:A:1290:ARG:NH1	2:A:1290:ARG:HG2	2.03	0.73
2:A:1531:THR:O	2:A:1534:VAL:CG2	2.37	0.73
2:A:196:ILE:HD12	2:A:197:VAL:N	2.03	0.73
2:A:855:LEU:CD2	2:A:1331:PHE:HE2	1.87	0.73
2:A:936:MET:CE	2:A:945:LEU:CD1	2.67	0.73
2:A:1500:PRO:HG3	2:A:1505:GLN:HG2	1.70	0.73
2:A:415:GLU:OE2	2:A:416:ALA:N	2.22	0.72
2:A:145:MET:HE2	2:A:145:MET:HA	1.69	0.72
2:A:224:THR:HA	2:A:227:VAL:CG2	2.20	0.72
2:A:1336:SER:O	2:A:1340:VAL:HG23	1.89	0.72
2:A:116:ARG:NH1	2:A:176:PHE:HB2	2.05	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:92:TRP:NE1	3:B:94:GLY:HA3	1.99	0.72
1:C:30:MET:HB3	1:C:138:GLY:HA2	1.71	0.72
1:C:65:LEU:HD12	1:C:110:VAL:CG1	2.19	0.72
3:B:104:LEU:HD12	3:B:104:LEU:N	2.03	0.72
2:A:410:GLN:HE21	2:A:410:GLN:C	1.92	0.72
2:A:1520:SER:O	2:A:1523:VAL:HG12	1.88	0.72
2:A:1214:ILE:HD12	3:B:22:VAL:CG2	2.18	0.72
2:A:1295:LEU:HD12	2:A:1298:LEU:CD2	1.95	0.72
2:A:1542:HIS:O	2:A:1546:VAL:HG23	1.90	0.72
3:B:141:LYS:HB3	3:B:141:LYS:NZ	2.01	0.72
1:C:71:GLU:HG3	1:C:94:ARG:HH12	1.53	0.72
2:A:142:PHE:HE1	2:A:152:THR:HG1	1.37	0.72
2:A:737:ILE:HD11	2:A:797:ALA:N	2.05	0.72
2:A:895:CYS:HB3	2:A:938:VAL:HG12	1.70	0.72
2:A:735:LYS:HZ2	2:A:739:PHE:HB2	1.46	0.72
2:A:1290:ARG:HG2	2:A:1290:ARG:HH11	1.54	0.72
2:A:1668:TYR:O	2:A:1729:ASP:HB2	1.89	0.72
3:B:54:PHE:CE2	3:B:124:TYR:HB2	2.25	0.72
2:A:737:ILE:HG13	2:A:738:TYR:H	1.54	0.72
2:A:145:MET:HA	2:A:145:MET:CE	2.19	0.71
2:A:318:SER:HB2	2:A:320:ASP:OD1	1.90	0.71
2:A:1265:ILE:HD12	2:A:1299:ARG:CG	2.20	0.71
1:C:33:THR:HB	1:C:51:THR:OG1	1.90	0.71
2:A:791:MET:CG	2:A:816:VAL:HG21	2.20	0.71
3:B:57:TRP:CZ3	3:B:142:ILE:HD11	2.25	0.71
3:B:69:LYS:NZ	3:B:81:GLU:OE1	2.22	0.71
1:C:41:LEU:HD23	1:C:147:LEU:HB3	1.71	0.71
2:A:174:ARG:CB	2:A:182:THR:HB	2.16	0.71
2:A:1322:MET:HA	2:A:1322:MET:CE	2.19	0.71
2:A:117:ARG:HA	2:A:120:ILE:HG22	1.73	0.71
2:A:305:TYR:CE1	2:A:311:ASP:HA	2.20	0.71
1:C:107:LYS:NZ	1:C:109:ASP:OD2	2.24	0.71
2:A:262:ILE:HG12	2:A:1617:ILE:HD12	1.73	0.71
2:A:181:PHE:O	2:A:185:ARG:HG2	1.91	0.71
2:A:184:LEU:HD12	2:A:190:TRP:CD1	2.26	0.71
2:A:290:MET:HE1	2:A:333:ILE:HG22	1.72	0.71
2:A:844:LYS:O	2:A:847:LYS:HE2	1.89	0.71
1:C:33:THR:HB	1:C:51:THR:HB	1.73	0.71
2:A:188:TRP:CD1	2:A:232:LYS:CE	2.74	0.71
2:A:245:LEU:HD13	2:A:249:MET:HE1	1.73	0.71
2:A:321:SER:HB2	2:A:372:ARG:O	1.91	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:327:GLY:O	3:B:132:TYR:CE2	2.43	0.71
2:A:855:LEU:O	2:A:859:ILE:HG13	1.91	0.71
2:A:1261:LEU:O	2:A:1265:ILE:HG12	1.91	0.71
2:A:811:PHE:CE1	2:A:815:ILE:CD1	2.69	0.70
2:A:899:ILE:CG2	2:A:934:ASP:OD2	2.37	0.70
2:A:1317:ALA:O	2:A:1321:ILE:HG12	1.91	0.70
2:A:1365:PRO:O	2:A:1424:GLN:HB3	1.91	0.70
2:A:1273:LEU:HD12	2:A:1273:LEU:O	1.91	0.70
2:A:817:THR:O	2:A:821:VAL:CG2	2.39	0.70
2:A:928:TRP:CZ3	2:A:929:ILE:CD1	2.74	0.70
2:A:960:LEU:CD2	2:A:964:LEU:CD2	2.66	0.70
2:A:795:LEU:HA	2:A:803:TYR:CD2	2.26	0.70
2:A:238:LEU:HD23	2:A:957:LEU:HD21	1.73	0.70
2:A:1353:THR:CG2	2:A:1379:ASN:O	2.39	0.70
2:A:1504:ILE:CD1	2:A:1505:GLN:H	2.03	0.70
2:A:293:LEU:CD1	2:A:298:ASP:C	2.60	0.70
2:A:1218:ARG:HG2	3:B:23:GLU:O	1.92	0.70
2:A:1268:VAL:HG13	2:A:1289:LEU:CD1	2.21	0.70
2:A:813:SER:HA	2:A:816:VAL:CG2	2.22	0.70
3:B:125:ARG:NH1	3:B:125:ARG:HG3	2.06	0.70
3:B:60:ARG:O	3:B:60:ARG:HG3	1.90	0.70
3:B:71:LEU:CD2	3:B:106:ILE:HD12	2.21	0.70
2:A:388:LEU:O	2:A:392:TYR:HB3	1.91	0.69
2:A:1221:THR:O	2:A:1224:ILE:HG22	1.92	0.69
2:A:1574:PHE:HD1	2:A:1580:ILE:CD1	2.04	0.69
2:A:936:MET:CE	2:A:945:LEU:CG	2.71	0.69
2:A:1485:MET:SD	2:A:1639:MET:HE1	2.31	0.69
2:A:1504:ILE:HD13	2:A:1505:GLN:N	2.05	0.69
3:B:104:LEU:N	3:B:104:LEU:CD1	2.53	0.69
2:A:291:ASN:HD22	2:A:292:THR:H	1.39	0.69
2:A:399:ALA:HB3	2:A:1762:ASN:ND2	2.07	0.69
3:B:112:THR:HG22	3:B:113:TYR:N	2.07	0.69
3:B:27:GLU:OE2	3:B:27:GLU:HA	1.92	0.69
2:A:1499:ARG:NH1	2:A:1501:GLY:HA2	2.07	0.69
2:A:1502:ASN:CB	2:A:1504:ILE:HD11	2.23	0.69
1:C:135:ARG:HG2	1:C:135:ARG:NH2	2.00	0.69
2:A:789:ALA:O	2:A:792:VAL:HG12	1.93	0.69
2:A:807:GLY:O	2:A:810:ILE:HG12	1.91	0.69
2:A:1650:LEU:HD13	2:A:1650:LEU:O	1.93	0.69
1:C:71:GLU:CG	1:C:94:ARG:HH12	2.05	0.69
2:A:291:ASN:HD22	2:A:292:THR:N	1.90	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:935:CYS:C	2:A:944:CYS:SG	2.71	0.69
2:A:1212:GLU:O	2:A:1663:MET:CE	2.40	0.69
2:A:1220:LYS:NZ	3:B:27:GLU:OE2	2.25	0.69
2:A:1430:SER:CB	2:A:1433:MET:HG2	2.23	0.69
3:B:67:PHE:CZ	3:B:120:GLU:OE2	2.45	0.69
3:B:70:ILE:O	3:B:81:GLU:N	2.23	0.69
3:B:71:LEU:HB3	3:B:80:LEU:HD12	1.66	0.69
3:B:71:LEU:CD2	3:B:106:ILE:CD1	2.70	0.69
2:A:123:LEU:HD23	2:A:123:LEU:O	1.92	0.69
2:A:736:CYS:O	2:A:740:ILE:N	2.25	0.69
2:A:286:LEU:C	2:A:286:LEU:HD23	2.14	0.68
2:A:328:TYR:CE1	3:B:132:TYR:HD2	2.11	0.68
2:A:862:SER:O	2:A:870:THR:CG2	2.39	0.68
2:A:1516:ALA:O	2:A:1520:SER:OG	2.10	0.68
2:A:1532:MET:CE	2:A:1620:ILE:CG1	2.70	0.68
2:A:153:LYS:HG3	2:A:157:TYR:CE2	2.28	0.68
2:A:1238:ILE:HD11	2:A:1270:LEU:HD23	0.75	0.68
2:A:1265:ILE:HD12	2:A:1299:ARG:HG2	1.74	0.68
3:B:166:LEU:O	3:B:170:LEU:HG	1.94	0.68
2:A:936:MET:HE3	2:A:945:LEU:HG	1.75	0.68
1:C:61:LYS:HG3	1:C:85:MET:CE	2.24	0.68
2:A:795:LEU:N	2:A:803:TYR:CD2	2.61	0.68
3:B:174:LEU:CD1	3:B:178:MET:SD	2.81	0.68
2:A:772:PHE:HE1	2:A:776:LEU:HD21	1.54	0.68
2:A:844:LYS:O	2:A:847:LYS:HD2	1.94	0.68
2:A:1283:LEU:HD23	2:A:1283:LEU:N	2.08	0.68
2:A:1504:ILE:HD11	2:A:1505:GLN:NE2	2.08	0.68
2:A:163:TYR:O	2:A:167:SER:OG	2.12	0.68
3:B:67:PHE:CE2	3:B:120:GLU:CD	2.67	0.68
1:C:33:THR:N	1:C:51:THR:O	2.27	0.68
2:A:160:THR:O	2:A:164:THR:HG23	1.94	0.68
3:B:125:ARG:HG3	3:B:125:ARG:HH11	1.59	0.68
2:A:1561:GLU:HG3	2:A:1562:CYS:N	2.07	0.68
2:A:191:LEU:C	2:A:191:LEU:HD23	2.14	0.67
2:A:336:ASN:HD21	2:A:343:SER:HB3	1.55	0.67
2:A:733:PHE:CE1	2:A:796:ILE:CG2	2.75	0.67
1:C:32:VAL:HG12	1:C:50:CYS:SG	2.33	0.67
1:C:82:GLN:HE22	5:C:301:NAG:C8	1.91	0.67
2:A:142:PHE:HE1	2:A:152:THR:OG1	1.76	0.67
2:A:207:LEU:CG	2:A:209:ASN:OD1	2.40	0.67
2:A:741:VAL:O	2:A:746:VAL:HG21	1.93	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:195:VAL:HG11	2:A:220:ARG:HG3	1.76	0.67
2:A:1500:PRO:HG3	2:A:1505:GLN:HB3	1.56	0.67
3:B:177:GLU:HA	3:B:177:GLU:OE1	1.94	0.67
1:C:65:LEU:C	1:C:65:LEU:HD23	2.15	0.67
3:B:50:ASN:O	3:B:50:ASN:ND2	2.28	0.67
2:A:136:ILE:C	2:A:136:ILE:HD13	2.15	0.67
2:A:737:ILE:HD13	2:A:796:ILE:HG22	1.75	0.67
2:A:842:VAL:O	2:A:845:LEU:HD12	1.94	0.67
2:A:1273:LEU:O	2:A:1277:THR:HB	1.94	0.67
3:B:92:TRP:CD1	3:B:94:GLY:N	2.62	0.67
2:A:224:THR:O	2:A:228:ILE:HD12	1.94	0.67
2:A:327:GLY:CA	3:B:134:HIS:CD2	2.78	0.67
2:A:967:LEU:C	2:A:967:LEU:HD23	2.15	0.67
1:C:34:VAL:HG23	1:C:142:ILE:HG12	1.76	0.67
3:B:72:ARG:NH2	3:B:74:GLU:CD	2.48	0.67
3:B:81:GLU:OE2	3:B:81:GLU:HA	1.95	0.67
2:A:168:LEU:HD23	2:A:168:LEU:C	2.14	0.67
3:B:85:ARG:O	3:B:115:HIS:HE1	1.78	0.67
2:A:264:LEU:O	2:A:268:MET:HB3	1.95	0.66
3:B:55:THR:CG2	3:B:104:LEU:HD23	2.26	0.66
2:A:171:ILE:HD12	2:A:171:ILE:C	2.15	0.66
2:A:226:SER:CB	2:A:232:LYS:NZ	2.59	0.66
2:A:737:ILE:CD1	2:A:797:ALA:N	2.58	0.66
2:A:765:HIS:HB2	2:A:767:PRO:HD2	1.77	0.66
2:A:881:ALA:O	2:A:916:SER:OG	2.13	0.66
2:A:1322:MET:HA	2:A:1322:MET:HE3	1.76	0.66
2:A:1431:LEU:HD12	2:A:1431:LEU:O	1.95	0.66
3:B:73:TYR:CD1	3:B:78:LEU:HB2	2.29	0.66
2:A:136:ILE:HD11	2:A:224:THR:HG21	1.77	0.66
2:A:1212:GLU:O	2:A:1663:MET:HE2	1.95	0.66
2:A:1389:PHE:CE1	2:A:1399:LEU:HD13	2.30	0.66
2:A:217:ARG:HB3	2:A:217:ARG:NH1	2.10	0.66
2:A:960:LEU:HD23	2:A:960:LEU:O	1.95	0.66
2:A:1764:SER:C	2:A:1767:THR:HG22	2.16	0.66
3:B:98:THR:O	3:B:99:LYS:HB3	1.95	0.66
2:A:131:LEU:HD13	2:A:131:LEU:C	2.15	0.66
2:A:971:PHE:HE2	2:A:1458:ASP:OD2	1.76	0.66
2:A:1600:GLU:OE1	2:A:1600:GLU:HA	1.95	0.66
1:C:65:LEU:CD1	1:C:110:VAL:CG1	2.74	0.66
2:A:116:ARG:HH12	2:A:176:PHE:HA	1.60	0.66
2:A:1202:ILE:O	2:A:1206:SER:OG	2.14	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:153:LYS:HE2	2:A:157:TYR:OH	1.96	0.66
2:A:332:LYS:HG3	2:A:332:LYS:O	1.94	0.66
2:A:388:LEU:HD13	2:A:388:LEU:C	2.16	0.66
2:A:1318:ILE:CG1	2:A:1319:PRO:HD3	2.26	0.66
2:A:238:LEU:O	2:A:241:SER:HB3	1.95	0.66
2:A:262:ILE:HG12	2:A:1617:ILE:CD1	2.26	0.66
2:A:1511:LEU:C	2:A:1511:LEU:HD23	2.15	0.66
3:B:92:TRP:HE1	3:B:94:GLY:C	1.99	0.66
2:A:226:SER:CB	2:A:232:LYS:HZ2	2.09	0.65
2:A:278:ASN:HD21	2:A:329:THR:N	1.94	0.65
2:A:849:TRP:HB3	2:A:852:LEU:HB2	1.77	0.65
2:A:1296:ARG:HD3	2:A:1299:ARG:HH21	1.62	0.65
2:A:1318:ILE:HG13	2:A:1319:PRO:HD3	1.76	0.65
2:A:1363:GLN:O	2:A:1364:VAL:HG12	1.96	0.65
2:A:1457:ILE:HG22	2:A:1756:ILE:HD12	1.76	0.65
2:A:1500:PRO:CB	2:A:1505:GLN:HB3	2.25	0.65
2:A:1732:ASN:HB3	2:A:1735:VAL:HG12	1.78	0.65
3:B:38:ILE:CG2	3:B:142:ILE:HD13	2.26	0.65
1:C:65:LEU:HD12	1:C:110:VAL:HG11	1.77	0.65
2:A:207:LEU:HD12	2:A:208:GLY:N	2.10	0.65
2:A:810:ILE:HG13	2:A:811:PHE:N	2.12	0.65
2:A:930:GLU:OE1	6:A:2007:9SR:O20	2.14	0.65
2:A:1282:ASP:HA	2:A:1286:ILE:HG21	1.77	0.65
2:A:321:SER:HB3	2:A:375:GLY:CA	2.26	0.65
2:A:726:CYS:HB2	2:A:728:PRO:HD2	1.79	0.65
2:A:1457:ILE:HD12	2:A:1457:ILE:C	2.16	0.65
2:A:844:LYS:O	2:A:847:LYS:HE3	1.94	0.65
2:A:1616:ARG:C	2:A:1618:GLY:N	2.48	0.65
2:A:742:MET:O	2:A:744:PRO:N	2.30	0.65
2:A:251:LEU:CD1	2:A:1630:ILE:HG21	2.25	0.65
2:A:336:ASN:CB	2:A:343:SER:OG	2.45	0.65
2:A:1430:SER:HG	2:A:1433:MET:HG2	1.57	0.65
3:B:92:TRP:HE1	3:B:94:GLY:CA	2.09	0.65
2:A:794:LYS:O	2:A:798:MET:HG2	1.97	0.65
2:A:847:LYS:H	2:A:847:LYS:CD	1.98	0.65
2:A:1251:LYS:O	2:A:1255:THR:CG2	2.40	0.64
2:A:226:SER:HB2	2:A:232:LYS:NZ	2.13	0.64
2:A:293:LEU:HD12	2:A:298:ASP:C	2.18	0.64
2:A:850:PRO:O	2:A:853:ASN:HB2	1.97	0.64
2:A:398:LEU:HD12	2:A:960:LEU:HD11	1.79	0.64
2:A:794:LYS:C	2:A:803:TYR:CD2	2.71	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:157:ILE:HD13	3:B:157:ILE:C	2.17	0.64
2:A:131:LEU:HD13	2:A:132:ILE:N	2.12	0.64
2:A:332:LYS:O	2:A:333:ILE:HG12	1.97	0.64
2:A:772:PHE:O	2:A:772:PHE:HD1	1.80	0.64
2:A:945:LEU:O	2:A:949:MET:HG2	1.97	0.64
2:A:1389:PHE:CZ	2:A:1399:LEU:CD1	2.81	0.64
2:A:1616:ARG:O	2:A:1617:ILE:C	2.34	0.64
3:B:73:TYR:HD1	3:B:78:LEU:HB2	1.62	0.64
2:A:909:HIS:CD2	2:A:911:ASN:H	2.16	0.64
2:A:947:VAL:O	2:A:951:VAL:HG23	1.98	0.64
2:A:1364:VAL:HG23	2:A:1370:CYS:HA	1.79	0.64
2:A:1279:GLY:O	2:A:1280:TYR:HB3	1.97	0.64
2:A:742:MET:O	2:A:744:PRO:CD	2.46	0.64
2:A:1385:LEU:O	2:A:1386:LYS:HB2	1.96	0.64
2:A:1499:ARG:HG3	2:A:1499:ARG:O	1.98	0.64
2:A:1528:ASN:HD22	2:A:1528:ASN:C	2.02	0.64
2:A:731:ILE:O	2:A:734:LYS:HB2	1.98	0.64
2:A:791:MET:O	2:A:791:MET:HE3	1.98	0.64
2:A:960:LEU:HD21	2:A:964:LEU:CD2	2.28	0.64
2:A:1491:LYS:O	2:A:1491:LYS:HD3	1.98	0.64
2:A:1650:LEU:HD13	2:A:1650:LEU:C	2.18	0.64
2:A:1694:ILE:CD1	2:A:1703:LEU:CD1	2.67	0.64
2:A:119:SER:OG	2:A:173:ALA:HB2	1.97	0.63
2:A:1295:LEU:O	2:A:1298:LEU:HB2	1.97	0.63
2:A:1760:LEU:HD23	2:A:1760:LEU:O	1.98	0.63
2:A:866:LEU:O	2:A:870:THR:HG22	1.97	0.63
2:A:1274:VAL:HA	2:A:1277:THR:CG2	2.27	0.63
2:A:166:GLU:HG3	2:A:167:SER:N	2.13	0.63
2:A:867:GLY:HA2	2:A:870:THR:CG2	2.28	0.63
2:A:117:ARG:CA	2:A:120:ILE:HG22	2.29	0.63
2:A:142:PHE:CE1	2:A:152:THR:OG1	2.51	0.63
2:A:1671:LYS:NZ	2:A:1682:GLU:OE2	2.32	0.63
2:A:1694:ILE:HD11	2:A:1700:TRP:HA	1.81	0.63
3:B:46:ARG:NH2	3:B:48:GLU:OE2	2.27	0.63
3:B:174:LEU:HD11	3:B:178:MET:SD	2.38	0.63
2:A:1407:GLY:O	2:A:1410:ILE:HG22	1.98	0.63
2:A:1647:ILE:CG2	2:A:1754:MET:HE3	2.28	0.63
2:A:1485:MET:SD	2:A:1639:MET:CE	2.87	0.63
2:A:1703:LEU:O	2:A:1706:PRO:HD2	1.98	0.63
2:A:1742:SER:O	2:A:1746:ILE:HG13	1.98	0.63
2:A:117:ARG:HA	2:A:120:ILE:CG2	2.28	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1639:MET:HE2	2:A:1639:MET:CA	2.29	0.63
2:A:209:ASN:HB2	2:A:212:ALA:HB3	1.80	0.63
2:A:1184:THR:HG23	3:B:181:CYS:HB3	1.80	0.63
2:A:360:GLN:NE2	2:A:390:SER:OG	2.32	0.62
2:A:1499:ARG:NE	2:A:1500:PRO:O	2.29	0.62
3:B:153:ASP:OD1	3:B:153:ASP:N	2.32	0.62
2:A:207:LEU:HD21	2:A:209:ASN:ND2	2.13	0.62
2:A:962:LEU:O	2:A:966:LEU:HB2	2.00	0.62
3:B:87:GLU:CD	3:B:88:GLY:N	2.51	0.62
2:A:290:MET:CE	2:A:333:ILE:CG2	2.77	0.62
2:A:835:ARG:O	2:A:837:PHE:N	2.32	0.62
2:A:960:LEU:HD23	2:A:964:LEU:CD2	2.22	0.62
2:A:1274:VAL:CA	2:A:1277:THR:HG22	2.29	0.62
2:A:1497:ILE:CG2	2:A:1572:TYR:CE2	2.76	0.62
2:A:117:ARG:HH11	2:A:117:ARG:CG	2.12	0.62
2:A:133:MET:O	2:A:136:ILE:HG23	2.00	0.62
2:A:153:LYS:CG	2:A:157:TYR:CE2	2.82	0.62
2:A:733:PHE:CE1	2:A:737:ILE:CG2	2.82	0.62
2:A:1647:ILE:HG22	2:A:1754:MET:HE3	1.81	0.62
1:C:56:TYR:HD1	2:A:898:LYS:HD2	1.64	0.62
2:A:1219:LYS:HG3	2:A:1219:LYS:O	2.00	0.62
2:A:160:THR:HG23	2:A:161:GLY:N	2.13	0.62
2:A:795:LEU:CA	2:A:803:TYR:CD2	2.83	0.62
1:C:34:VAL:CG2	1:C:142:ILE:HG12	2.29	0.61
2:A:760:PHE:CE2	2:A:779:GLY:HA3	2.34	0.61
3:B:85:ARG:HG2	3:B:85:ARG:HH11	1.65	0.61
2:A:251:LEU:HD12	2:A:1630:ILE:CG2	2.26	0.61
2:A:1752:VAL:O	2:A:1756:ILE:HG12	2.00	0.61
1:C:82:GLN:NE2	5:C:301:NAG:N2	2.47	0.61
2:A:1367:ARG:HB2	2:A:1382:TRP:CZ2	2.36	0.61
2:A:1408:TRP:NE1	2:A:1409:THR:HG22	2.16	0.61
2:A:1502:ASN:HB3	2:A:1504:ILE:HD12	1.81	0.61
3:B:174:LEU:O	3:B:178:MET:HG2	2.00	0.61
2:A:349:TRP:HA	2:A:349:TRP:CE3	2.36	0.61
2:A:743:ASP:N	2:A:744:PRO:HD2	2.14	0.61
2:A:902:ASP:OD2	2:A:902:ASP:N	2.31	0.61
1:C:105:PRO:HA	1:C:109:ASP:O	2.01	0.61
3:B:55:THR:HG21	3:B:104:LEU:HD23	1.82	0.61
1:C:59:ASN:O	1:C:63:PHE:N	2.30	0.61
2:A:148:PRO:CB	2:A:152:THR:HG21	2.28	0.61
2:A:178:VAL:HG12	2:A:178:VAL:O	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:210:VAL:O	2:A:213:LEU:HD22	1.99	0.61
2:A:1531:THR:O	2:A:1534:VAL:HG23	2.00	0.61
1:C:65:LEU:HD21	1:C:67:TRP:CD1	2.35	0.61
3:B:57:TRP:HZ3	3:B:142:ILE:CD1	2.12	0.61
1:C:62:GLN:C	1:C:132:PRO:HD2	2.21	0.61
1:C:103:GLY:HA3	1:C:109:ASP:OD1	1.99	0.61
3:B:26:SER:OG	3:B:142:ILE:CG2	2.44	0.61
2:A:737:ILE:CD1	2:A:797:ALA:CA	2.78	0.61
3:B:53:THR:HG22	3:B:54:PHE:N	2.15	0.61
2:A:198:PHE:O	2:A:202:THR:N	2.30	0.60
2:A:1230:ASP:OD1	2:A:1296:ARG:NH2	2.33	0.60
2:A:1318:ILE:HG13	2:A:1319:PRO:CD	2.29	0.60
2:A:171:ILE:CG2	2:A:183:PHE:CD2	2.75	0.60
2:A:936:MET:HE1	2:A:945:LEU:HD11	1.82	0.60
2:A:967:LEU:HD23	2:A:968:LEU:N	2.16	0.60
3:B:31:VAL:CG2	3:B:150:ALA:HB2	2.30	0.60
3:B:85:ARG:HH11	3:B:85:ARG:CG	2.14	0.60
2:A:849:TRP:CE3	2:A:852:LEU:CD2	2.83	0.60
3:B:51:ALA:HB2	3:B:127:LEU:HA	1.83	0.60
3:B:91:VAL:HG21	3:B:107:PHE:HD2	1.67	0.60
2:A:1707:ILE:HG21	2:A:1736:GLY:HA3	1.83	0.60
3:B:40:CYS:O	3:B:104:LEU:O	2.19	0.60
3:B:55:THR:HG22	3:B:56:GLU:N	2.16	0.60
2:A:931:THR:HG22	2:A:948:TYR:OH	2.01	0.60
2:A:1505:GLN:O	2:A:1509:PHE:HB3	2.00	0.60
3:B:91:VAL:HG22	3:B:107:PHE:O	2.02	0.60
2:A:735:LYS:HZ2	2:A:739:PHE:CB	2.04	0.60
2:A:1628:LYS:HD2	2:A:1628:LYS:C	2.22	0.60
3:B:65:GLU:OE2	3:B:65:GLU:N	2.34	0.60
2:A:207:LEU:CD2	2:A:209:ASN:OD1	2.49	0.60
2:A:967:LEU:HD22	2:A:968:LEU:HD13	1.83	0.60
2:A:791:MET:SD	2:A:816:VAL:HG21	2.42	0.60
2:A:791:MET:HE3	2:A:791:MET:C	2.22	0.60
2:A:791:MET:HE3	2:A:795:LEU:HD21	1.82	0.60
2:A:814:LEU:O	2:A:817:THR:OG1	2.19	0.60
2:A:1502:ASN:HB2	2:A:1504:ILE:HD11	1.84	0.60
2:A:133:MET:O	2:A:136:ILE:CG2	2.50	0.59
2:A:1405:PHE:HE1	2:A:1441:ILE:HD13	1.67	0.59
2:A:1509:PHE:CB	2:A:1568:SER:HB3	2.31	0.59
3:B:55:THR:OG1	3:B:104:LEU:HD21	2.00	0.59
2:A:936:MET:CE	2:A:945:LEU:HD12	2.31	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1179:TRP:CD1	2:A:1183:LYS:HE2	2.37	0.59
1:C:55:CYS:SG	2:A:898:LYS:HD3	2.42	0.59
2:A:1218:ARG:CG	3:B:23:GLU:O	2.50	0.59
2:A:1389:PHE:HE1	2:A:1399:LEU:HD13	1.66	0.59
2:A:1504:ILE:HD11	2:A:1505:GLN:HE21	1.67	0.59
2:A:201:LEU:O	2:A:204:PHE:O	2.19	0.59
2:A:1304:PHE:CD2	2:A:1307:MET:CE	2.85	0.59
2:A:1512:VAL:HA	2:A:1517:PHE:HD2	1.67	0.59
2:A:855:LEU:CG	2:A:1331:PHE:HE2	2.16	0.59
2:A:1364:VAL:O	2:A:1364:VAL:HG13	2.00	0.59
3:B:175:VAL:O	3:B:179:ILE:HG12	2.02	0.59
2:A:1499:ARG:NH1	2:A:1501:GLY:O	2.35	0.59
2:A:1572:TYR:O	2:A:1575:THR:HG23	2.03	0.59
2:A:174:ARG:HD3	2:A:182:THR:CB	2.29	0.59
2:A:936:MET:HE2	2:A:945:LEU:HD12	1.84	0.59
2:A:1293:ARG:HB3	2:A:1293:ARG:NH2	2.15	0.59
2:A:1450:ASN:HD22	2:A:1450:ASN:C	2.06	0.59
3:B:125:ARG:HH11	3:B:125:ARG:CG	2.15	0.59
2:A:251:LEU:HD12	2:A:1630:ILE:HG21	1.84	0.59
2:A:336:ASN:HD22	2:A:343:SER:HB3	1.61	0.59
2:A:798:MET:O	2:A:799:ASP:HB2	2.03	0.59
2:A:1281:SER:O	2:A:1282:ASP:HB2	2.02	0.59
2:A:1764:SER:O	2:A:1767:THR:CG2	2.41	0.59
2:A:1704:LEU:HD22	2:A:1708:LEU:HG	1.84	0.58
2:A:293:LEU:CD1	2:A:298:ASP:O	2.51	0.58
2:A:337:PRO:O	2:A:338:ASP:HB2	2.02	0.58
2:A:1318:ILE:N	2:A:1319:PRO:HD2	2.18	0.58
2:A:1440:PHE:O	2:A:1444:GLY:N	2.33	0.58
1:C:65:LEU:HD21	1:C:67:TRP:HD1	1.67	0.58
2:A:795:LEU:CD2	2:A:795:LEU:H	2.07	0.58
2:A:928:TRP:HZ3	2:A:929:ILE:CD1	2.12	0.58
2:A:737:ILE:CD1	2:A:796:ILE:HG22	2.33	0.58
2:A:1522:MET:HE3	2:A:1522:MET:O	2.04	0.58
3:B:89:ARG:HH11	3:B:89:ARG:CG	2.16	0.58
3:B:129:PHE:HB2	3:B:132:TYR:HB3	1.85	0.58
2:A:861:ASN:O	2:A:866:LEU:HB2	2.04	0.58
2:A:896:VAL:O	2:A:898:LYS:N	2.36	0.58
2:A:1412:MET:HE2	2:A:1434:TYR:CE1	2.38	0.58
2:A:1496:PRO:O	2:A:1497:ILE:CG1	2.51	0.58
2:A:1509:PHE:O	2:A:1512:VAL:HG23	2.04	0.58
2:A:213:LEU:HD23	2:A:214:ARG:CG	2.31	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1343:PHE:HE2	2:A:1436:TYR:CE2	2.20	0.58
2:A:1616:ARG:HH11	2:A:1616:ARG:CG	2.14	0.58
2:A:136:ILE:CG1	2:A:224:THR:HG22	2.34	0.58
2:A:1416:VAL:HG11	2:A:1434:TYR:CE2	2.39	0.58
3:B:70:ILE:O	3:B:81:GLU:HB2	2.02	0.58
2:A:1179:TRP:NE1	2:A:1183:LYS:HE2	2.19	0.58
2:A:1200:LEU:HD23	2:A:1201:MET:CE	2.34	0.58
2:A:1485:MET:CB	2:A:1639:MET:CE	2.81	0.58
2:A:1500:PRO:HG3	2:A:1505:GLN:HG3	1.84	0.58
2:A:1504:ILE:HD13	2:A:1504:ILE:N	2.17	0.58
2:A:166:GLU:OE2	2:A:223:LYS:NZ	2.36	0.58
2:A:389:GLY:O	2:A:393:LEU:HB2	2.03	0.58
2:A:1500:PRO:CG	2:A:1505:GLN:HG2	2.30	0.58
2:A:361:ASP:OD2	2:A:929:ILE:CG2	2.50	0.58
2:A:367:TYR:OH	2:A:1689:ILE:CG2	2.50	0.58
2:A:383:VAL:O	2:A:387:PHE:HB2	2.04	0.58
2:A:737:ILE:HD13	2:A:796:ILE:CG2	2.34	0.58
2:A:895:CYS:O	2:A:896:VAL:C	2.40	0.58
2:A:1318:ILE:CG1	2:A:1319:PRO:CD	2.82	0.58
2:A:1431:LEU:HD12	2:A:1431:LEU:C	2.24	0.57
2:A:1497:ILE:HG21	2:A:1572:TYR:CD2	2.24	0.57
2:A:895:CYS:HB2	2:A:938:VAL:HG12	1.85	0.57
2:A:1603:PHE:CD1	2:A:1603:PHE:N	2.73	0.57
3:B:51:ALA:CB	3:B:127:LEU:HD13	2.30	0.57
2:A:133:MET:HA	2:A:136:ILE:CG2	2.35	0.57
2:A:967:LEU:HD23	2:A:968:LEU:HD13	1.82	0.57
2:A:290:MET:CE	2:A:333:ILE:HG22	2.33	0.57
2:A:1389:PHE:CE1	2:A:1399:LEU:CD1	2.88	0.57
2:A:1740:PHE:O	2:A:1744:ILE:HG12	2.04	0.57
3:B:37:LYS:HB2	3:B:107:PHE:HD1	1.69	0.57
1:C:65:LEU:HD23	1:C:65:LEU:O	2.04	0.57
2:A:414:GLU:HG3	2:A:415:GLU:N	2.19	0.57
3:B:66:GLU:C	3:B:67:PHE:HD1	2.08	0.57
2:A:363:TRP:CZ3	2:A:367:TYR:CB	2.88	0.57
2:A:794:LYS:HB3	2:A:803:TYR:HE2	0.59	0.57
2:A:813:SER:O	2:A:816:VAL:HG23	2.05	0.57
2:A:1506:GLY:O	2:A:1510:ASP:OD1	2.23	0.57
2:A:196:ILE:CD1	2:A:197:VAL:CG2	2.80	0.57
2:A:792:VAL:HG13	2:A:793:LEU:N	2.18	0.57
3:B:51:ALA:CB	3:B:126:LEU:O	2.53	0.57
2:A:363:TRP:HZ3	2:A:367:TYR:CB	2.17	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:855:LEU:HD23	2:A:1331:PHE:CE2	2.31	0.56
2:A:1359:PHE:HB3	2:A:1360:PRO:HD2	1.85	0.56
2:A:1716:ASP:OD1	2:A:1717:PRO:CD	2.47	0.56
3:B:46:ARG:HB3	3:B:48:GLU:OE2	2.05	0.56
2:A:1264:LEU:O	2:A:1268:VAL:HG23	2.05	0.56
2:A:1358:ARG:NH1	2:A:1417:ASP:OD2	2.36	0.56
3:B:57:TRP:CZ3	3:B:142:ILE:CD1	2.86	0.56
2:A:1185:CYS:O	2:A:1189:VAL:HG22	2.04	0.56
2:A:1206:SER:O	2:A:1209:LEU:HB2	2.05	0.56
2:A:1531:THR:O	2:A:1534:VAL:HG22	2.04	0.56
1:C:101:PHE:CZ	1:C:103:GLY:O	2.56	0.56
2:A:157:TYR:C	2:A:160:THR:HG22	2.20	0.56
2:A:1427:TYR:CD2	2:A:1428:GLU:HB2	2.40	0.56
2:A:1637:LEU:HD22	2:A:1637:LEU:O	2.05	0.56
2:A:320:ASP:OD1	2:A:320:ASP:N	2.39	0.56
2:A:791:MET:HE1	2:A:795:LEU:HD11	1.87	0.56
2:A:1334:ILE:HG22	2:A:1338:MET:CE	2.36	0.56
2:A:1358:ARG:NH2	2:A:1417:ASP:OD2	2.38	0.56
3:B:80:LEU:HD21	3:B:90:VAL:HB	1.87	0.56
2:A:336:ASN:ND2	2:A:343:SER:OG	2.38	0.56
2:A:840:LEU:O	2:A:843:PHE:CD2	2.59	0.56
3:B:65:GLU:H	3:B:65:GLU:CD	2.09	0.56
2:A:116:ARG:O	2:A:120:ILE:HG22	2.06	0.56
2:A:226:SER:CB	2:A:232:LYS:HE3	2.36	0.56
2:A:1500:PRO:CB	2:A:1505:GLN:HG2	2.36	0.56
2:A:1508:ILE:HD13	2:A:1567:ILE:HG21	1.87	0.56
2:A:898:LYS:O	2:A:899:ILE:HG23	2.05	0.56
2:A:1532:MET:HE3	2:A:1620:ILE:CG1	2.35	0.56
2:A:1551:ASN:OD1	2:A:1619:ARG:NH1	2.39	0.56
3:B:31:VAL:HG21	3:B:150:ALA:HB2	1.87	0.56
1:C:107:LYS:O	1:C:108:TYR:HB2	2.06	0.56
1:C:137:ARG:NH2	5:C:301:NAG:C6	2.68	0.56
2:A:1504:ILE:O	2:A:1508:ILE:HD12	2.06	0.56
2:A:225:ILE:HA	2:A:231:LEU:HD23	1.87	0.56
2:A:395:ASN:OD1	2:A:1755:TYR:CD1	2.59	0.56
2:A:839:LEU:O	2:A:842:VAL:HG23	2.04	0.56
2:A:794:LYS:C	2:A:803:TYR:HD2	2.07	0.55
2:A:795:LEU:CD2	2:A:795:LEU:N	2.65	0.55
2:A:838:ARG:O	2:A:841:ARG:HG3	2.05	0.55
2:A:1498:PRO:HD2	2:A:1572:TYR:CE2	2.41	0.55
2:A:1669:VAL:HA	2:A:1729:ASP:O	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:85:ARG:NH1	3:B:85:ARG:HB3	2.21	0.55
3:B:93:ASN:OD1	3:B:107:PHE:HB2	2.05	0.55
2:A:139:ASN:C	2:A:139:ASN:HD22	2.07	0.55
2:A:787:PHE:N	2:A:787:PHE:CD1	2.73	0.55
2:A:1589:SER:OG	2:A:1619:ARG:NH2	2.40	0.55
1:C:44:SER:O	1:C:117:VAL:HG22	2.07	0.55
2:A:188:TRP:CE2	2:A:232:LYS:HE2	2.40	0.55
2:A:1616:ARG:C	2:A:1618:GLY:H	2.08	0.55
3:B:82:GLU:O	3:B:82:GLU:HG3	2.06	0.55
2:A:1755:TYR:CD1	2:A:1755:TYR:N	2.75	0.55
2:A:1304:PHE:HB2	2:A:1307:MET:HE3	1.87	0.55
2:A:132:ILE:HD11	2:A:166:GLU:HB2	1.87	0.55
2:A:305:TYR:HE1	2:A:311:ASP:C	2.05	0.55
2:A:1321:ILE:HD11	2:A:1456:ILE:HG12	1.89	0.55
2:A:908:TRP:HE1	2:A:1413:TYR:HH	1.52	0.55
2:A:1717:PRO:HG2	2:A:1718:LYS:HZ2	1.71	0.55
2:A:849:TRP:HE3	2:A:852:LEU:CD2	2.19	0.55
2:A:896:VAL:CG2	2:A:897:CYS:H	2.05	0.55
2:A:1214:ILE:HD12	3:B:22:VAL:HG23	1.88	0.55
2:A:1265:ILE:HD12	2:A:1299:ARG:HG3	1.88	0.55
2:A:1293:ARG:HD2	2:A:1296:ARG:NH2	2.21	0.55
2:A:1304:PHE:CD2	2:A:1307:MET:HE3	2.42	0.55
2:A:1408:TRP:CD1	2:A:1409:THR:HG23	2.42	0.55
2:A:1640:SER:HB3	2:A:1761:GLU:HG3	1.89	0.55
3:B:157:ILE:HG23	3:B:158:VAL:N	2.22	0.55
1:C:32:VAL:HG13	1:C:50:CYS:SG	2.44	0.55
1:C:66:ASN:ND2	1:C:79:MET:HE1	2.14	0.55
2:A:116:ARG:NH1	2:A:176:PHE:CB	2.65	0.55
2:A:1681:PHE:HD1	2:A:1687:SER:HG	1.52	0.55
3:B:71:LEU:CB	3:B:80:LEU:HD11	2.33	0.54
2:A:249:MET:CE	2:A:249:MET:CA	2.85	0.54
2:A:737:ILE:HD12	2:A:797:ALA:HB2	1.87	0.54
2:A:840:LEU:CD1	2:A:843:PHE:HE2	2.08	0.54
2:A:293:LEU:HD11	2:A:298:ASP:C	2.26	0.54
2:A:772:PHE:CE1	2:A:776:LEU:CD2	2.89	0.54
2:A:1707:ILE:HD13	2:A:1740:PHE:CE2	2.42	0.54
2:A:1389:PHE:HZ	2:A:1399:LEU:CD1	2.21	0.54
3:B:144:ILE:HG13	3:B:144:ILE:O	2.06	0.54
2:A:192:ASP:OD2	2:A:223:LYS:HD2	2.07	0.54
2:A:196:ILE:HD11	2:A:197:VAL:HG23	1.89	0.54
2:A:286:LEU:CD1	2:A:331:VAL:HG21	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1647:ILE:CG2	2:A:1754:MET:HE1	2.30	0.54
2:A:1668:TYR:O	2:A:1729:ASP:CA	2.54	0.54
2:A:1694:ILE:CD1	2:A:1700:TRP:HA	2.38	0.54
3:B:48:GLU:HG2	3:B:49:THR:N	2.22	0.54
1:C:33:THR:O	1:C:50:CYS:CA	2.55	0.54
1:C:59:ASN:HB3	1:C:62:GLN:CB	2.34	0.54
3:B:85:ARG:O	3:B:115:HIS:CE1	2.59	0.54
3:B:85:ARG:CZ	3:B:85:ARG:CB	2.86	0.54
2:A:166:GLU:O	2:A:169:VAL:HG22	2.08	0.54
2:A:282:ASN:N	2:A:282:ASN:HD22	2.04	0.54
2:A:1546:VAL:HG12	2:A:1550:ILE:HD11	1.90	0.54
1:C:62:GLN:HB3	1:C:132:PRO:HD2	1.90	0.54
2:A:155:VAL:HG12	2:A:159:PHE:CE2	2.43	0.54
2:A:160:THR:CG2	2:A:161:GLY:N	2.70	0.54
2:A:1270:LEU:HD13	2:A:1270:LEU:C	2.26	0.54
2:A:1290:ARG:HH11	2:A:1290:ARG:CG	2.17	0.54
2:A:1322:MET:CE	2:A:1322:MET:CA	2.85	0.54
3:B:71:LEU:CD2	3:B:106:ILE:HD11	2.37	0.54
1:C:107:LYS:O	1:C:107:LYS:HG2	2.08	0.53
1:C:135:ARG:HH21	1:C:135:ARG:CG	2.15	0.53
2:A:262:ILE:CG1	2:A:1617:ILE:CD1	2.86	0.53
2:A:1186:TYR:CZ	2:A:1190:GLU:OE2	2.62	0.53
2:A:814:LEU:HA	2:A:817:THR:OG1	2.08	0.53
2:A:1524:LEU:HD22	2:A:1554:PHE:HE1	1.72	0.53
2:A:146:ASN:O	2:A:147:ASN:HB3	2.08	0.53
2:A:823:LEU:HD12	2:A:823:LEU:O	2.08	0.53
2:A:867:GLY:O	2:A:870:THR:HG23	2.09	0.53
2:A:1211:PHE:O	2:A:1216:ILE:HD13	2.07	0.53
2:A:1212:GLU:O	2:A:1663:MET:HE1	2.08	0.53
2:A:132:ILE:CD1	2:A:166:GLU:CB	2.79	0.53
2:A:329:THR:HG22	2:A:330:CYS:N	2.23	0.53
2:A:1350:CYS:HB2	2:A:1424:GLN:HE22	1.74	0.53
2:A:810:ILE:HG13	2:A:811:PHE:H	1.72	0.53
2:A:847:LYS:HD2	2:A:847:LYS:N	2.11	0.53
2:A:1232:ILE:HD12	3:B:166:LEU:HD12	1.91	0.53
2:A:1696:THR:O	2:A:1697:SER:OG	2.15	0.53
2:A:123:LEU:HD23	2:A:123:LEU:C	2.29	0.53
2:A:808:TRP:CD1	2:A:811:PHE:HD2	2.26	0.53
2:A:1343:PHE:HE2	2:A:1436:TYR:HE2	1.56	0.53
2:A:145:MET:CE	2:A:145:MET:CA	2.85	0.53
2:A:238:LEU:HD23	2:A:957:LEU:CD2	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:277:ARG:CG	2:A:302:TYR:O	2.56	0.53
2:A:772:PHE:CD1	2:A:776:LEU:HD21	2.43	0.53
2:A:803:TYR:CZ	2:A:809:ASN:OD1	2.62	0.53
2:A:1304:PHE:HD2	2:A:1307:MET:HE3	1.72	0.53
2:A:1477:GLU:OE2	2:A:1477:GLU:HA	2.07	0.53
2:A:791:MET:HG3	2:A:816:VAL:CG2	2.34	0.53
2:A:824:PHE:O	2:A:825:LEU:HD12	2.09	0.53
3:B:91:VAL:HG21	3:B:107:PHE:CD2	2.44	0.53
3:B:174:LEU:HD13	3:B:174:LEU:C	2.29	0.53
2:A:163:TYR:CE2	2:A:220:ARG:HG2	2.37	0.52
2:A:217:ARG:CB	2:A:217:ARG:CZ	2.86	0.52
2:A:1495:LYS:CA	2:A:1495:LYS:HE3	2.39	0.52
2:A:153:LYS:HG2	2:A:157:TYR:HE2	1.73	0.52
2:A:303:PHE:CD1	2:A:303:PHE:N	2.76	0.52
2:A:795:LEU:HD22	2:A:803:TYR:CE1	2.44	0.52
2:A:803:TYR:CE1	2:A:809:ASN:CG	2.83	0.52
2:A:837:PHE:CD1	2:A:840:LEU:HD23	2.45	0.52
2:A:1265:ILE:CD1	2:A:1299:ARG:HG2	2.40	0.52
2:A:1365:PRO:O	2:A:1424:GLN:CB	2.58	0.52
2:A:1408:TRP:NE1	2:A:1409:THR:CG2	2.73	0.52
2:A:1495:LYS:CA	2:A:1495:LYS:CE	2.86	0.52
2:A:1595:LEU:O	2:A:1599:ILE:CD1	2.50	0.52
2:A:1232:ILE:CD1	3:B:166:LEU:HD12	2.40	0.52
2:A:1495:LYS:CE	2:A:1495:LYS:HA	2.38	0.52
2:A:1647:ILE:HG22	2:A:1754:MET:HE1	1.88	0.52
2:A:1694:ILE:HG13	2:A:1703:LEU:CD1	2.40	0.52
3:B:91:VAL:CG2	3:B:107:PHE:HD2	2.23	0.52
1:C:137:ARG:NH2	5:C:301:NAG:H62	2.25	0.52
2:A:114:PRO:HG2	2:A:115:LEU:H	1.74	0.52
2:A:1412:MET:HE2	2:A:1434:TYR:HE1	1.74	0.52
2:A:1504:ILE:CD1	2:A:1504:ILE:N	2.73	0.52
2:A:1733:PRO:O	2:A:1737:ILE:HG13	2.10	0.52
1:C:47:ARG:NH2	1:C:111:SER:OG	2.43	0.52
2:A:114:PRO:O	2:A:118:ILE:HG12	2.09	0.52
2:A:195:VAL:HG11	2:A:220:ARG:CG	2.38	0.52
2:A:812:ASP:O	2:A:816:VAL:HG22	2.08	0.52
2:A:1532:MET:CE	2:A:1620:ILE:HG13	2.39	0.52
3:B:58:THR:HG22	3:B:69:LYS:CA	2.39	0.52
3:B:154:MET:O	3:B:158:VAL:HG23	2.09	0.52
3:B:174:LEU:O	3:B:178:MET:CG	2.58	0.52
2:A:175:GLY:O	2:A:178:VAL:HB	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:184:LEU:HD12	2:A:190:TRP:NE1	2.25	0.52
2:A:278:ASN:HD21	2:A:329:THR:CB	2.21	0.52
2:A:314:LEU:O	2:A:372:ARG:HD3	2.10	0.52
3:B:149:LYS:O	3:B:151:ASN:ND2	2.43	0.52
2:A:176:PHE:O	2:A:178:VAL:HG23	2.08	0.52
2:A:793:LEU:HD13	2:A:793:LEU:O	2.10	0.52
2:A:1677:ASP:OD1	2:A:1677:ASP:C	2.45	0.52
2:A:397:ILE:O	2:A:401:VAL:HG23	2.09	0.52
2:A:890:LYS:NZ	2:A:890:LYS:CB	2.73	0.52
2:A:1457:ILE:CG2	2:A:1756:ILE:HD11	2.25	0.52
2:A:1504:ILE:CD1	2:A:1505:GLN:NE2	2.73	0.52
3:B:54:PHE:CE1	3:B:124:TYR:CD2	2.87	0.52
2:A:220:ARG:O	2:A:223:LYS:HB2	2.10	0.52
2:A:245:LEU:CD1	2:A:249:MET:HE1	2.39	0.52
2:A:338:ASP:O	2:A:339:TYR:HB2	2.10	0.52
2:A:757:ASN:OD1	2:A:841:ARG:NH1	2.42	0.52
2:A:1349:GLU:HG3	2:A:1351:ILE:CG2	2.40	0.52
3:B:112:THR:CG2	3:B:113:TYR:N	2.73	0.52
2:A:415:GLU:OE2	2:A:416:ALA:HB2	2.09	0.51
2:A:746:VAL:O	2:A:750:ILE:HG12	2.10	0.51
2:A:1668:TYR:O	2:A:1729:ASP:HA	2.10	0.51
2:A:144:THR:O	2:A:144:THR:HG22	2.10	0.51
2:A:1467:LEU:HD11	2:A:1472:ILE:CG2	2.41	0.51
2:A:290:MET:HE2	2:A:333:ILE:CG2	2.40	0.51
2:A:1473:PHE:O	2:A:1646:ASN:ND2	2.37	0.51
2:A:1485:MET:CB	2:A:1639:MET:HE3	2.24	0.51
3:B:85:ARG:NH1	3:B:85:ARG:CB	2.73	0.51
1:C:79:MET:HE2	5:C:301:NAG:C1	2.37	0.51
2:A:1504:ILE:CD1	2:A:1505:GLN:HE21	2.24	0.51
2:A:1611:VAL:O	2:A:1614:LEU:HB2	2.11	0.51
2:A:217:ARG:CG	2:A:217:ARG:HH11	2.24	0.51
2:A:289:ILE:HD12	2:A:302:TYR:CZ	2.46	0.51
2:A:936:MET:HE1	2:A:945:LEU:HG	1.89	0.51
2:A:1519:ILE:CD1	2:A:1519:ILE:N	2.73	0.51
2:A:772:PHE:CD1	2:A:776:LEU:CD2	2.93	0.51
2:A:849:TRP:CH2	2:A:1326:LEU:HB3	2.46	0.51
2:A:851:THR:O	2:A:852:LEU:C	2.49	0.51
2:A:1298:LEU:CD1	2:A:1301:LEU:CD1	2.86	0.51
2:A:195:VAL:CG1	2:A:220:ARG:HG3	2.39	0.51
2:A:272:LYS:NZ	2:A:345:ASP:OD2	2.44	0.51
2:A:737:ILE:CG1	2:A:738:TYR:N	2.73	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:831:LEU:N	2:A:831:LEU:CD2	2.73	0.51
2:A:1340:VAL:O	2:A:1344:ALA:HB2	2.11	0.51
2:A:152:THR:HA	2:A:155:VAL:HG23	1.92	0.51
2:A:1707:ILE:HD13	2:A:1740:PHE:HE2	1.74	0.51
1:C:30:MET:HB3	1:C:138:GLY:CA	2.40	0.51
2:A:795:LEU:N	2:A:803:TYR:CE2	2.79	0.51
2:A:851:THR:O	2:A:854:MET:N	2.43	0.51
2:A:1190:GLU:HA	2:A:1190:GLU:OE1	2.11	0.51
2:A:117:ARG:CG	2:A:117:ARG:NH1	2.73	0.50
2:A:217:ARG:NH1	2:A:217:ARG:CB	2.73	0.50
2:A:238:LEU:CD2	2:A:957:LEU:CD2	2.89	0.50
2:A:743:ASP:N	2:A:744:PRO:CD	2.74	0.50
2:A:1282:ASP:CA	2:A:1286:ILE:HG21	2.41	0.50
1:C:107:LYS:HZ3	1:C:109:ASP:HB2	1.62	0.50
2:A:209:ASN:HB2	2:A:212:ALA:CB	2.41	0.50
2:A:822:GLU:OE1	2:A:835:ARG:HD3	2.11	0.50
2:A:1527:LEU:O	2:A:1530:VAL:HG12	2.11	0.50
2:A:1573:TYR:OH	2:A:1583:PHE:HB2	2.11	0.50
2:A:1680:ASN:O	2:A:1686:ASN:HB3	2.11	0.50
2:A:405:TYR:CD1	2:A:405:TYR:C	2.85	0.50
2:A:758:THR:HA	2:A:761:MET:HE2	1.92	0.50
2:A:811:PHE:C	2:A:811:PHE:CD1	2.85	0.50
2:A:1605:SER:HB3	2:A:1608:LEU:HB3	1.93	0.50
2:A:1212:GLU:OE1	2:A:1293:ARG:NH1	2.44	0.50
2:A:1668:TYR:CE1	2:A:1721:HIS:ND1	2.73	0.50
3:B:92:TRP:CE2	3:B:94:GLY:N	2.80	0.50
2:A:825:LEU:HD12	2:A:825:LEU:N	2.27	0.50
2:A:1408:TRP:CD1	2:A:1409:THR:CG2	2.94	0.50
2:A:1613:ARG:O	2:A:1616:ARG:HD3	2.11	0.50
2:A:151:TRP:CE3	2:A:152:THR:HA	2.47	0.50
2:A:297:GLU:HA	2:A:297:GLU:OE2	2.12	0.50
2:A:823:LEU:HD12	2:A:823:LEU:C	2.32	0.50
2:A:1474:MET:HE1	2:A:1482:TYR:CD1	2.45	0.50
3:B:32:TYR:CD1	3:B:32:TYR:C	2.84	0.50
3:B:60:ARG:NH1	3:B:67:PHE:CE1	2.80	0.50
2:A:133:MET:HA	2:A:136:ILE:HG22	1.93	0.50
2:A:813:SER:CA	2:A:816:VAL:HG23	2.39	0.50
2:A:1755:TYR:N	2:A:1755:TYR:HD1	2.07	0.50
1:C:137:ARG:NH2	5:C:301:NAG:H61	2.27	0.50
2:A:117:ARG:O	2:A:120:ILE:HG22	2.12	0.50
2:A:151:TRP:CE3	2:A:151:TRP:C	2.85	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:869:LEU:HD12	2:A:869:LEU:C	2.32	0.50
2:A:1502:ASN:HB3	2:A:1504:ILE:HD11	1.85	0.50
2:A:1527:LEU:O	2:A:1530:VAL:CG1	2.58	0.50
2:A:1548:TYR:CD1	2:A:1548:TYR:C	2.85	0.50
1:C:34:VAL:HG21	1:C:142:ILE:HG13	1.93	0.50
2:A:1213:ASP:HB3	2:A:1663:MET:HE1	1.89	0.50
3:B:174:LEU:HD13	3:B:178:MET:HG2	1.94	0.50
2:A:737:ILE:CD1	2:A:797:ALA:HB2	2.42	0.49
2:A:1360:PRO:O	2:A:1361:ALA:HB3	2.12	0.49
2:A:1292:LEU:O	2:A:1295:LEU:HB2	2.12	0.49
2:A:1416:VAL:HA	2:A:1430:SER:HB3	1.94	0.49
2:A:1506:GLY:O	2:A:1510:ASP:OD2	2.28	0.49
3:B:66:GLU:C	3:B:67:PHE:CD1	2.85	0.49
3:B:129:PHE:HB2	3:B:132:TYR:O	2.12	0.49
2:A:293:LEU:HD12	2:A:298:ASP:CA	2.42	0.49
2:A:729:TYR:C	2:A:729:TYR:CD1	2.86	0.49
2:A:803:TYR:CD1	2:A:803:TYR:C	2.85	0.49
2:A:1369:GLU:OE1	2:A:1369:GLU:HA	2.12	0.49
2:A:1408:TRP:CD1	2:A:1409:THR:N	2.80	0.49
2:A:1467:LEU:HD21	2:A:1472:ILE:CG2	2.42	0.49
2:A:1574:PHE:CD1	2:A:1580:ILE:CD1	2.91	0.49
3:B:112:THR:HG22	3:B:113:TYR:H	1.74	0.49
2:A:131:LEU:HD22	2:A:131:LEU:C	2.33	0.49
2:A:755:VAL:HG13	2:A:756:LEU:N	2.27	0.49
2:A:1551:ASN:O	2:A:1555:ILE:HG13	2.11	0.49
2:A:1717:PRO:HG2	2:A:1718:LYS:NZ	2.28	0.49
3:B:26:SER:HB2	3:B:39:LEU:H	1.78	0.49
1:C:128:TYR:HB3	1:C:137:ARG:HE	1.76	0.49
2:A:183:PHE:C	2:A:183:PHE:CD1	2.85	0.49
2:A:209:ASN:CB	2:A:212:ALA:HB3	2.42	0.49
2:A:251:LEU:HD11	2:A:1634:LEU:CD2	2.41	0.49
2:A:293:LEU:HD11	2:A:298:ASP:O	2.13	0.49
2:A:349:TRP:HA	2:A:349:TRP:HE3	1.78	0.49
2:A:742:MET:CA	2:A:744:PRO:HD2	2.42	0.49
2:A:1283:LEU:N	2:A:1283:LEU:CD2	2.73	0.49
2:A:1505:GLN:O	2:A:1509:PHE:CB	2.60	0.49
1:C:52:PHE:CD1	1:C:52:PHE:C	2.85	0.49
2:A:125:HIS:ND1	2:A:126:SER:N	2.60	0.49
2:A:757:ASN:O	2:A:757:ASN:ND2	2.45	0.49
2:A:765:HIS:CD2	2:A:768:MET:CG	2.96	0.49
2:A:1602:TYR:C	2:A:1603:PHE:CD1	2.86	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:151:ASN:ND2	3:B:151:ASN:N	2.60	0.49
3:B:84:GLU:OE1	3:B:84:GLU:N	2.45	0.49
1:C:54:SER:HB2	1:C:134:ASP:OD2	2.13	0.49
2:A:1427:TYR:CD2	2:A:1427:TYR:C	2.85	0.49
2:A:1627:ALA:HB3	2:A:1630:ILE:HD11	1.75	0.49
2:A:1640:SER:CB	2:A:1761:GLU:HG3	2.42	0.49
2:A:1667:ALA:O	2:A:1668:TYR:HB2	2.13	0.49
3:B:85:ARG:CG	3:B:85:ARG:NH1	2.73	0.49
3:B:126:LEU:HD13	3:B:128:PHE:CE1	2.46	0.49
1:C:34:VAL:CG2	1:C:142:ILE:CG1	2.91	0.49
1:C:61:LYS:HG3	1:C:85:MET:HE1	1.94	0.49
2:A:281:GLU:O	2:A:282:ASN:HB2	2.13	0.49
2:A:1318:ILE:HG13	2:A:1319:PRO:N	2.28	0.49
2:A:1333:LEU:O	2:A:1337:ILE:HG13	2.12	0.49
2:A:1509:PHE:CD1	2:A:1509:PHE:C	2.85	0.49
4:E:2:NAG:HO3	4:E:2:NAG:C7	2.17	0.49
2:A:116:ARG:NH2	2:A:176:PHE:HB2	2.28	0.48
2:A:363:TRP:HZ3	2:A:367:TYR:CG	2.30	0.48
2:A:879:ILE:O	2:A:882:VAL:HG12	2.12	0.48
3:B:57:TRP:CH2	3:B:142:ILE:HD11	2.48	0.48
1:C:34:VAL:CG1	1:C:50:CYS:SG	2.96	0.48
2:A:117:ARG:HB3	2:A:117:ARG:NH1	2.17	0.48
2:A:117:ARG:C	2:A:120:ILE:HG22	2.32	0.48
2:A:911:ASN:HD22	2:A:911:ASN:C	2.12	0.48
2:A:1404:THR:O	2:A:1405:PHE:HB2	2.13	0.48
2:A:1500:PRO:CB	2:A:1505:GLN:CB	2.87	0.48
2:A:1502:ASN:HB2	2:A:1504:ILE:CD1	2.41	0.48
2:A:1573:TYR:CD1	2:A:1573:TYR:C	2.85	0.48
2:A:249:MET:HE2	2:A:249:MET:N	2.28	0.48
2:A:766:HIS:CD2	2:A:766:HIS:C	2.86	0.48
2:A:807:GLY:HA2	2:A:810:ILE:HG12	1.95	0.48
3:B:60:ARG:NH1	3:B:67:PHE:HE1	2.11	0.48
1:C:128:TYR:CE2	1:C:137:ARG:NH2	2.74	0.48
2:A:217:ARG:O	2:A:220:ARG:HD3	2.14	0.48
2:A:370:THR:HG21	2:A:382:PHE:HZ	1.77	0.48
2:A:1503:LYS:O	2:A:1507:CYS:N	2.30	0.48
2:A:1639:MET:CE	2:A:1639:MET:CA	2.85	0.48
2:A:1760:LEU:HD23	2:A:1760:LEU:C	2.33	0.48
2:A:277:ARG:HD3	2:A:302:TYR:HA	1.95	0.48
2:A:339:TYR:HB2	2:A:341:TYR:CD2	2.49	0.48
2:A:374:ALA:HB1	2:A:378:TYR:CD2	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1635:PHE:C	2:A:1635:PHE:CD1	2.85	0.48
2:A:890:LYS:HZ3	2:A:890:LYS:HB3	1.76	0.48
2:A:1373:LEU:O	2:A:1377:SER:HB2	2.13	0.48
2:A:1694:ILE:HD12	2:A:1703:LEU:HD12	1.81	0.48
2:A:226:SER:CB	2:A:232:LYS:CE	2.91	0.48
2:A:741:VAL:HG23	2:A:743:ASP:H	1.79	0.48
2:A:811:PHE:CZ	2:A:815:ILE:HD11	2.42	0.48
2:A:963:PHE:CD1	2:A:963:PHE:C	2.87	0.48
2:A:1321:ILE:CD1	2:A:1456:ILE:HG12	2.42	0.48
2:A:1456:ILE:HG21	2:A:1752:VAL:HG11	1.95	0.48
1:C:34:VAL:HG21	1:C:142:ILE:CG1	2.43	0.48
2:A:249:MET:CA	2:A:249:MET:HE2	2.44	0.48
2:A:922:ARG:NH1	2:A:927:GLU:OE1	2.39	0.48
2:A:1261:LEU:O	2:A:1261:LEU:HD12	2.13	0.48
2:A:336:ASN:HD22	2:A:343:SER:CB	2.20	0.48
2:A:791:MET:SD	2:A:813:SER:OG	2.65	0.48
2:A:899:ILE:HD12	2:A:934:ASP:OD2	2.14	0.48
2:A:1191:HIS:ND1	2:A:1192:SER:N	2.61	0.48
2:A:1694:ILE:HG13	2:A:1703:LEU:HD11	1.96	0.48
3:B:55:THR:CB	3:B:104:LEU:HD23	2.43	0.48
2:A:336:ASN:HB2	2:A:343:SER:OG	2.11	0.47
2:A:1504:ILE:CG1	2:A:1505:GLN:N	2.77	0.47
1:C:59:ASN:CB	1:C:62:GLN:CB	2.85	0.47
2:A:116:ARG:HH22	2:A:176:PHE:HB2	1.79	0.47
2:A:1274:VAL:O	2:A:1278:LEU:CB	2.62	0.47
2:A:1709:ASN:HB2	2:A:1714:ASP:CB	2.41	0.47
1:C:61:LYS:HA	1:C:85:MET:SD	2.54	0.47
2:A:168:LEU:HD23	2:A:169:VAL:CA	2.42	0.47
2:A:277:ARG:HG2	2:A:302:TYR:O	2.14	0.47
2:A:1459:ASN:O	2:A:1459:ASN:ND2	2.48	0.47
2:A:1574:PHE:CD1	2:A:1580:ILE:HD11	2.36	0.47
2:A:1694:ILE:CG1	2:A:1703:LEU:HD12	2.39	0.47
2:A:214:ARG:O	2:A:217:ARG:HG2	2.15	0.47
2:A:839:LEU:N	2:A:839:LEU:HD22	2.29	0.47
2:A:1242:LEU:O	2:A:1246:ILE:HG12	2.15	0.47
2:A:1467:LEU:HD11	2:A:1472:ILE:HG23	1.96	0.47
2:A:251:LEU:HD11	2:A:1634:LEU:HD22	1.95	0.47
2:A:251:LEU:HB2	2:A:1630:ILE:HG23	1.95	0.47
2:A:363:TRP:HZ3	2:A:367:TYR:HB2	1.78	0.47
2:A:736:CYS:O	2:A:739:PHE:HB3	2.14	0.47
2:A:1254:PHE:HD1	2:A:1260:TRP:CE2	2.32	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1289:LEU:HD22	2:A:1292:LEU:HD23	1.97	0.47
2:A:1637:LEU:HD22	2:A:1637:LEU:C	2.34	0.47
2:A:276:PHE:HB2	2:A:331:VAL:CG1	2.45	0.47
2:A:735:LYS:O	2:A:739:PHE:HB3	2.14	0.47
2:A:1215:TYR:CE1	3:B:22:VAL:HG22	2.49	0.47
2:A:1296:ARG:HD3	2:A:1299:ARG:NH2	2.29	0.47
4:E:1:NAG:H82	4:E:1:NAG:C1	2.44	0.47
1:C:34:VAL:HG23	1:C:35:PRO:N	2.29	0.47
1:C:55:CYS:SG	2:A:898:LYS:CD	3.02	0.47
2:A:116:ARG:CZ	2:A:176:PHE:HB2	2.44	0.47
2:A:273:HIS:O	2:A:314:LEU:HD12	2.13	0.47
2:A:321:SER:OG	2:A:322:GLY:N	2.48	0.47
2:A:322:GLY:HA3	2:A:323:GLN:HG2	1.95	0.47
2:A:849:TRP:HH2	2:A:1326:LEU:HB3	1.80	0.47
2:A:890:LYS:CB	2:A:890:LYS:HZ3	2.28	0.47
2:A:1710:SER:O	2:A:1711:LYS:HG2	2.14	0.47
2:A:1729:ASP:OD1	2:A:1729:ASP:N	2.41	0.47
3:B:53:THR:CG2	3:B:54:PHE:N	2.77	0.47
3:B:54:PHE:CE2	3:B:124:TYR:CB	2.96	0.47
3:B:55:THR:CG2	3:B:56:GLU:N	2.77	0.47
3:B:69:LYS:O	3:B:81:GLU:HG2	2.14	0.47
2:A:114:PRO:CG	2:A:115:LEU:H	2.27	0.47
2:A:226:SER:HB2	2:A:232:LYS:CE	2.45	0.47
2:A:245:LEU:HD13	2:A:249:MET:HE3	1.92	0.47
2:A:847:LYS:CD	2:A:847:LYS:N	2.73	0.47
2:A:945:LEU:HD23	2:A:949:MET:CE	2.45	0.47
2:A:1220:LYS:NZ	3:B:27:GLU:CD	2.68	0.47
2:A:1613:ARG:HG2	2:A:1616:ARG:HE	1.79	0.47
2:A:132:ILE:CD1	2:A:166:GLU:HB3	2.28	0.47
2:A:147:ASN:HD22	2:A:147:ASN:C	2.18	0.47
2:A:1293:ARG:HH21	2:A:1293:ARG:CG	2.28	0.47
2:A:1412:MET:CE	2:A:1434:TYR:CD1	2.98	0.47
2:A:171:ILE:HD12	2:A:172:LEU:N	2.30	0.47
2:A:206:ASN:OD1	2:A:206:ASN:N	2.48	0.47
2:A:1369:GLU:CG	4:E:1:NAG:H62	2.44	0.47
2:A:1504:ILE:CD1	2:A:1504:ILE:H	2.27	0.47
3:B:157:ILE:HD13	3:B:157:ILE:O	2.15	0.47
2:A:262:ILE:HG13	2:A:1617:ILE:HD13	1.98	0.46
2:A:831:LEU:N	2:A:831:LEU:HD22	2.30	0.46
2:A:836:SER:O	2:A:839:LEU:HD23	2.14	0.46
2:A:896:VAL:O	2:A:899:ILE:N	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:936:MET:HE1	2:A:945:LEU:CG	2.38	0.46
2:A:1179:TRP:HE1	2:A:1183:LYS:HE2	1.80	0.46
2:A:1420:ASN:HB3	2:A:1423:LYS:HG3	1.98	0.46
1:C:56:TYR:HA	2:A:898:LYS:HD2	1.96	0.46
2:A:1298:LEU:HD13	2:A:1657:ILE:HD11	1.97	0.46
2:A:151:TRP:HZ3	2:A:155:VAL:HG21	1.80	0.46
2:A:1289:LEU:O	2:A:1292:LEU:HB2	2.16	0.46
2:A:1304:PHE:CD2	2:A:1307:MET:HE1	2.50	0.46
2:A:1430:SER:OG	2:A:1433:MET:CE	2.63	0.46
3:B:51:ALA:CB	3:B:127:LEU:HA	2.44	0.46
2:A:176:PHE:HD2	2:A:178:VAL:HG21	1.80	0.46
2:A:1394:LEU:HD23	2:A:1394:LEU:HA	1.76	0.46
2:A:1419:VAL:HG12	2:A:1425:PRO:HA	1.96	0.46
2:A:794:LYS:HG3	2:A:798:MET:SD	2.56	0.46
2:A:843:PHE:O	2:A:845:LEU:N	2.48	0.46
2:A:899:ILE:HG21	2:A:934:ASP:CG	2.31	0.46
2:A:1524:LEU:HD23	2:A:1524:LEU:HA	1.79	0.46
2:A:133:MET:SD	2:A:133:MET:C	2.94	0.46
2:A:204:PHE:O	2:A:205:VAL:C	2.53	0.46
2:A:399:ALA:O	2:A:403:MET:HB2	2.15	0.46
2:A:741:VAL:O	2:A:746:VAL:HB	2.14	0.46
2:A:954:ILE:O	2:A:958:VAL:HG23	2.16	0.46
2:A:971:PHE:CD1	2:A:971:PHE:C	2.89	0.46
2:A:1273:LEU:HD12	2:A:1277:THR:HB	1.97	0.46
2:A:1349:GLU:HG3	2:A:1351:ILE:HG22	1.98	0.46
2:A:1424:GLN:HE21	2:A:1424:GLN:HB2	1.63	0.46
2:A:153:LYS:HG2	2:A:157:TYR:CE2	2.49	0.46
2:A:259:PHE:HB2	2:A:354:LEU:HD22	1.97	0.46
2:A:259:PHE:HB3	2:A:354:LEU:HD21	1.97	0.46
2:A:293:LEU:HD11	2:A:299:PHE:HA	1.98	0.46
2:A:792:VAL:CG1	2:A:793:LEU:N	2.78	0.46
2:A:837:PHE:CD1	2:A:840:LEU:CD2	2.99	0.46
2:A:956:ASN:N	2:A:956:ASN:HD22	2.14	0.46
2:A:1318:ILE:HG12	2:A:1319:PRO:HD3	1.96	0.46
2:A:1364:VAL:CG2	2:A:1370:CYS:HA	2.46	0.46
2:A:333:ILE:HG22	2:A:334:GLY:N	2.30	0.46
2:A:1366:ASN:OD1	2:A:1366:ASN:N	2.45	0.46
2:A:140:CYS:HA	2:A:143:MET:HG3	1.97	0.46
2:A:1274:VAL:O	2:A:1278:LEU:HB3	2.16	0.46
3:B:128:PHE:CD1	3:B:128:PHE:N	2.84	0.46
2:A:1304:PHE:HD2	2:A:1307:MET:CE	2.28	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:38:ILE:HG22	3:B:142:ILE:HD13	1.98	0.46
2:A:278:ASN:ND2	2:A:329:THR:N	2.64	0.45
2:A:807:GLY:C	2:A:810:ILE:HG12	2.35	0.45
2:A:1408:TRP:CZ3	2:A:1441:ILE:HD11	2.51	0.45
2:A:1497:ILE:HG12	2:A:1572:TYR:HB3	1.98	0.45
3:B:75:ASN:HB3	3:B:76:GLU:H	1.65	0.45
3:B:173:TRP:O	3:B:177:GLU:HB2	2.15	0.45
2:A:200:TYR:N	2:A:200:TYR:CD1	2.84	0.45
2:A:741:VAL:O	2:A:746:VAL:CB	2.64	0.45
2:A:760:PHE:HZ	2:A:775:VAL:HG12	1.81	0.45
2:A:1641:LEU:HA	2:A:1641:LEU:HD23	1.73	0.45
1:C:55:CYS:O	1:C:56:TYR:CG	2.70	0.45
2:A:398:LEU:CD1	2:A:960:LEU:HD11	2.45	0.45
2:A:1184:THR:CG2	3:B:181:CYS:HB3	2.47	0.45
2:A:1306:GLY:O	2:A:1309:VAL:HG12	2.17	0.45
2:A:1722:PRO:HB3	3:B:103:ASP:HB2	1.98	0.45
3:B:54:PHE:CD2	3:B:124:TYR:HB2	2.51	0.45
2:A:217:ARG:O	2:A:220:ARG:CD	2.64	0.45
2:A:395:ASN:ND2	2:A:1755:TYR:CE1	2.84	0.45
2:A:1364:VAL:HG23	2:A:1370:CYS:CA	2.46	0.45
3:B:91:VAL:CG2	3:B:107:PHE:CD2	3.00	0.45
2:A:188:TRP:CG	2:A:232:LYS:NZ	2.84	0.45
2:A:209:ASN:CG	2:A:212:ALA:HB3	2.36	0.45
2:A:300:ARG:HG3	2:A:305:TYR:CD2	2.51	0.45
2:A:745:PHE:O	2:A:749:ALA:HB2	2.17	0.45
2:A:852:LEU:HD13	2:A:852:LEU:HA	1.87	0.45
2:A:1301:LEU:CD2	2:A:1311:VAL:HG21	2.46	0.45
2:A:1471:ASP:OD1	2:A:1472:ILE:N	2.50	0.45
2:A:1571:HIS:CD2	2:A:1571:HIS:H	2.33	0.45
3:B:60:ARG:HB3	3:B:66:GLU:O	2.17	0.45
3:B:174:LEU:CD1	3:B:178:MET:CG	2.94	0.45
2:A:147:ASN:HD22	2:A:147:ASN:N	2.14	0.45
2:A:896:VAL:O	2:A:899:ILE:HG12	2.17	0.45
2:A:909:HIS:HD2	2:A:911:ASN:N	2.07	0.45
2:A:1273:LEU:HD12	2:A:1273:LEU:C	2.35	0.45
2:A:1430:SER:O	2:A:1432:TYR:N	2.47	0.45
2:A:1522:MET:HB3	2:A:1522:MET:HE2	1.70	0.45
2:A:1681:PHE:HD1	2:A:1687:SER:OG	1.99	0.45
3:B:101:LEU:O	3:B:103:ASP:N	2.43	0.45
3:B:114:ASN:OD1	5:B:303:NAG:O5	2.33	0.45
2:A:137:LEU:HD12	2:A:137:LEU:HA	1.79	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:147:ASN:C	2:A:147:ASN:ND2	2.70	0.45
2:A:388:LEU:O	2:A:388:LEU:HD13	2.15	0.45
2:A:732:LYS:HB2	2:A:732:LYS:HE3	1.66	0.45
3:B:38:ILE:HG21	3:B:142:ILE:HD13	1.97	0.45
3:B:64:THR:HG22	3:B:65:GLU:N	2.31	0.45
1:C:55:CYS:C	1:C:56:TYR:CG	2.90	0.45
2:A:332:LYS:C	2:A:333:ILE:HG12	2.37	0.45
2:A:890:LYS:NZ	2:A:890:LYS:HB3	2.30	0.45
2:A:1179:TRP:CD1	2:A:1183:LYS:CE	2.99	0.45
2:A:1343:PHE:HB3	2:A:1347:PHE:CE1	2.51	0.45
2:A:1513:THR:HG22	2:A:1513:THR:O	2.17	0.45
3:B:67:PHE:CE2	3:B:120:GLU:OE2	2.69	0.45
2:A:123:LEU:C	2:A:123:LEU:CD2	2.86	0.45
2:A:733:PHE:CD1	2:A:733:PHE:C	2.90	0.45
2:A:1369:GLU:HG2	4:E:1:NAG:H62	1.99	0.45
2:A:1530:VAL:HA	2:A:1533:MET:HG3	1.99	0.45
2:A:823:LEU:O	2:A:824:PHE:CD1	2.70	0.45
2:A:1274:VAL:O	2:A:1277:THR:HG22	2.17	0.45
2:A:1431:LEU:C	2:A:1431:LEU:CD1	2.86	0.45
2:A:1491:LYS:C	2:A:1491:LYS:CD	2.86	0.45
2:A:1499:ARG:NH1	2:A:1500:PRO:O	2.49	0.45
2:A:1326:LEU:HD22	2:A:1326:LEU:HA	1.85	0.44
2:A:1509:PHE:HB2	2:A:1568:SER:CB	2.39	0.44
3:B:46:ARG:HH21	3:B:48:GLU:CD	2.14	0.44
2:A:121:LYS:HB2	2:A:121:LYS:HE3	1.59	0.44
2:A:193:PHE:O	2:A:196:ILE:HG13	2.16	0.44
2:A:779:GLY:O	2:A:783:PHE:CD2	2.70	0.44
2:A:1355:ASP:OD1	2:A:1355:ASP:N	2.50	0.44
2:A:1444:GLY:O	2:A:1448:THR:OG1	2.32	0.44
3:B:59:PHE:CZ	3:B:61:GLN:HA	2.52	0.44
1:C:107:LYS:CD	1:C:109:ASP:HB2	2.41	0.44
2:A:739:PHE:O	2:A:739:PHE:CD1	2.70	0.44
2:A:1760:LEU:C	2:A:1760:LEU:CD2	2.86	0.44
3:B:174:LEU:CD1	3:B:174:LEU:C	2.86	0.44
2:A:116:ARG:NH1	2:A:176:PHE:HA	2.29	0.44
2:A:964:LEU:HD13	2:A:964:LEU:HA	1.80	0.44
2:A:1757:ALA:O	2:A:1761:GLU:HG2	2.18	0.44
2:A:176:PHE:O	2:A:176:PHE:CG	2.70	0.44
2:A:244:LYS:HE2	2:A:244:LYS:HB3	1.64	0.44
2:A:825:LEU:N	2:A:825:LEU:CD1	2.79	0.44
2:A:1270:LEU:C	2:A:1270:LEU:CD1	2.85	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1289:LEU:HD22	2:A:1289:LEU:HA	1.86	0.44
2:A:1704:LEU:HD22	2:A:1704:LEU:O	2.17	0.44
3:B:38:ILE:HB	3:B:106:ILE:HG22	1.99	0.44
1:C:56:TYR:CE1	2:A:895:CYS:HA	2.52	0.44
2:A:163:TYR:O	2:A:166:GLU:HG3	2.18	0.44
2:A:272:LYS:O	2:A:274:LYS:HG3	2.17	0.44
2:A:282:ASN:N	2:A:282:ASN:ND2	2.66	0.44
2:A:737:ILE:CG1	2:A:738:TYR:H	2.27	0.44
2:A:971:PHE:HD1	2:A:972:SER:HB2	1.83	0.44
2:A:1710:SER:O	2:A:1711:LYS:HE3	2.17	0.44
1:C:56:TYR:HE1	2:A:895:CYS:HA	1.82	0.44
1:C:58:VAL:HG13	1:C:63:PHE:CB	2.46	0.44
2:A:174:ARG:CD	2:A:182:THR:HG21	2.16	0.44
2:A:219:LEU:O	2:A:222:LEU:HB2	2.18	0.44
2:A:737:ILE:HA	2:A:740:ILE:HB	1.98	0.44
2:A:763:MET:O	2:A:764:GLU:HG2	2.16	0.44
2:A:1460:PHE:HD2	2:A:1756:ILE:HG13	1.82	0.44
2:A:1650:LEU:C	2:A:1650:LEU:CD1	2.86	0.44
1:C:55:CYS:O	1:C:56:TYR:CD2	2.70	0.44
2:A:164:THR:HG21	2:A:200:TYR:HH	1.80	0.44
2:A:213:LEU:HD23	2:A:214:ARG:CA	2.48	0.44
2:A:249:MET:HE2	2:A:249:MET:HA	1.99	0.44
2:A:1722:PRO:CB	3:B:103:ASP:HB2	2.47	0.44
1:C:34:VAL:HG23	1:C:35:PRO:O	2.18	0.44
1:C:128:TYR:HD2	1:C:137:ARG:NE	2.12	0.44
1:C:131:ASN:O	1:C:134:ASP:N	2.51	0.44
2:A:155:VAL:O	2:A:159:PHE:CD2	2.70	0.44
2:A:855:LEU:HG	2:A:1331:PHE:HE2	1.83	0.44
2:A:1437:PHE:O	2:A:1441:ILE:HG13	2.18	0.44
2:A:1496:PRO:C	2:A:1497:ILE:CG1	2.85	0.44
2:A:1499:ARG:NH1	2:A:1501:GLY:CA	2.73	0.44
2:A:1569:LEU:HB2	2:A:1573:TYR:HB2	2.00	0.44
2:A:1668:TYR:O	2:A:1729:ASP:HB3	2.13	0.44
3:B:66:GLU:O	3:B:67:PHE:CD1	2.71	0.44
2:A:136:ILE:HD13	2:A:137:LEU:N	2.33	0.43
2:A:410:GLN:HA	2:A:413:ILE:HG22	1.99	0.43
2:A:823:LEU:C	2:A:823:LEU:CD1	2.86	0.43
2:A:867:GLY:HA2	2:A:870:THR:HG22	2.00	0.43
2:A:911:ASN:O	2:A:911:ASN:ND2	2.40	0.43
2:A:1467:LEU:HD21	2:A:1472:ILE:HG22	1.99	0.43
2:A:1509:PHE:N	2:A:1568:SER:OG	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1566:LEU:HA	2:A:1566:LEU:HD12	1.75	0.43
2:A:1189:VAL:HG11	2:A:1244:LYS:HD3	2.00	0.43
2:A:1427:TYR:CE2	2:A:1428:GLU:HB2	2.52	0.43
2:A:1495:LYS:HE3	2:A:1495:LYS:N	2.33	0.43
2:A:1609:PHE:O	2:A:1609:PHE:CD1	2.70	0.43
2:A:153:LYS:HE3	2:A:157:TYR:HH	1.77	0.43
2:A:249:MET:CE	2:A:249:MET:HA	2.48	0.43
2:A:742:MET:O	2:A:744:PRO:HD2	2.04	0.43
2:A:1647:ILE:HD13	2:A:1753:ASN:HB3	2.00	0.43
1:C:55:CYS:SG	1:C:56:TYR:N	2.92	0.43
1:C:101:PHE:CZ	1:C:105:PRO:HD3	2.54	0.43
2:A:196:ILE:HG13	2:A:196:ILE:H	1.63	0.43
2:A:314:LEU:HD12	2:A:314:LEU:HA	1.87	0.43
2:A:361:ASP:OD2	2:A:929:ILE:CB	2.66	0.43
2:A:396:LEU:HD23	2:A:396:LEU:HA	1.76	0.43
2:A:1200:LEU:HD23	2:A:1201:MET:HE2	2.00	0.43
2:A:1314:LEU:O	2:A:1318:ILE:HG23	2.17	0.43
3:B:186:ALA:O	3:B:189:THR:OG1	2.28	0.43
1:C:61:LYS:HG3	1:C:85:MET:SD	2.58	0.43
2:A:156:GLU:OE1	2:A:217:ARG:NH2	2.50	0.43
2:A:835:ARG:C	2:A:837:PHE:H	2.22	0.43
2:A:1457:ILE:HD12	2:A:1458:ASP:CA	2.48	0.43
2:A:1504:ILE:CD1	2:A:1505:GLN:N	2.73	0.43
2:A:1764:SER:HA	2:A:1767:THR:HG22	2.01	0.43
2:A:252:THR:O	2:A:256:LEU:HG	2.19	0.43
2:A:899:ILE:CD1	2:A:934:ASP:OD2	2.66	0.43
2:A:1302:SER:O	2:A:1308:ARG:NH2	2.52	0.43
2:A:1317:ALA:CB	2:A:1459:ASN:OD1	2.66	0.43
2:A:1321:ILE:CD1	2:A:1456:ILE:CG1	2.97	0.43
3:B:112:THR:CG2	3:B:113:TYR:H	2.32	0.43
2:A:217:ARG:HH11	2:A:217:ARG:HG2	1.84	0.43
2:A:300:ARG:HA	2:A:305:TYR:HD2	1.84	0.43
2:A:305:TYR:CD1	2:A:311:ASP:C	2.92	0.43
2:A:363:TRP:CZ3	2:A:367:TYR:HB2	2.54	0.43
2:A:765:HIS:CD2	2:A:768:MET:HG3	2.54	0.43
2:A:801:TYR:O	2:A:801:TYR:CD1	2.72	0.43
2:A:1602:TYR:HB2	2:A:1603:PHE:CE1	2.53	0.43
2:A:1675:ILE:HD12	2:A:1706:PRO:HG3	2.01	0.43
2:A:1675:ILE:HD12	2:A:1706:PRO:CG	2.49	0.43
2:A:1763:PHE:O	2:A:1767:THR:HB	2.18	0.43
2:A:169:VAL:HG23	2:A:170:LYS:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:835:ARG:C	2:A:837:PHE:N	2.72	0.43
2:A:1628:LYS:C	2:A:1628:LYS:CD	2.86	0.43
2:A:1732:ASN:HB3	2:A:1735:VAL:CG1	2.47	0.43
3:B:71:LEU:HB3	3:B:80:LEU:HD11	1.91	0.43
2:A:151:TRP:CE3	2:A:152:THR:N	2.87	0.43
2:A:882:VAL:O	2:A:886:GLN:HG2	2.18	0.43
1:C:58:VAL:CG1	1:C:63:PHE:HB2	2.46	0.43
2:A:251:LEU:O	2:A:255:CYS:HB2	2.19	0.43
2:A:346:THR:HG22	2:A:347:PHE:N	2.34	0.43
2:A:971:PHE:HE2	2:A:1458:ASP:HB2	1.84	0.43
3:B:71:LEU:HD22	3:B:106:ILE:HD11	2.00	0.43
1:C:40:VAL:HG22	1:C:44:SER:OG	2.19	0.42
2:A:1317:ALA:HA	2:A:1459:ASN:OD1	2.19	0.42
3:B:26:SER:HG	3:B:142:ILE:HG21	1.79	0.42
3:B:146:VAL:HG12	3:B:147:VAL:N	2.32	0.42
2:A:737:ILE:C	2:A:739:PHE:N	2.72	0.42
2:A:741:VAL:O	2:A:746:VAL:HG23	2.17	0.42
2:A:764:GLU:C	2:A:765:HIS:ND1	2.73	0.42
2:A:1388:ASN:OD1	2:A:1394:LEU:HD13	2.19	0.42
2:A:1764:SER:HA	2:A:1767:THR:CG2	2.49	0.42
2:A:327:GLY:CA	3:B:134:HIS:NE2	2.81	0.42
2:A:806:VAL:HB	2:A:809:ASN:HB2	2.00	0.42
2:A:1504:ILE:C	2:A:1508:ILE:HD12	2.39	0.42
1:C:41:LEU:HD21	1:C:147:LEU:HD22	2.00	0.42
2:A:338:ASP:OD2	2:A:342:THR:OG1	2.29	0.42
2:A:380:ILE:O	2:A:384:VAL:HG12	2.19	0.42
2:A:399:ALA:HB1	2:A:1762:ASN:HD22	1.55	0.42
2:A:794:LYS:C	2:A:803:TYR:CE2	2.92	0.42
2:A:1373:LEU:O	2:A:1377:SER:N	2.52	0.42
3:B:101:LEU:N	3:B:101:LEU:HD13	2.33	0.42
2:A:139:ASN:C	2:A:139:ASN:ND2	2.73	0.42
2:A:415:GLU:CD	2:A:416:ALA:N	2.73	0.42
2:A:1496:PRO:O	2:A:1497:ILE:CB	2.67	0.42
2:A:1499:ARG:NH1	2:A:1501:GLY:C	2.73	0.42
3:B:89:ARG:CG	3:B:89:ARG:NH1	2.74	0.42
2:A:170:LYS:HE3	2:A:170:LYS:HB2	1.56	0.42
2:A:807:GLY:CA	2:A:810:ILE:HG12	2.50	0.42
2:A:1420:ASN:CB	2:A:1423:LYS:HG3	2.50	0.42
3:B:65:GLU:N	3:B:65:GLU:CD	2.73	0.42
3:B:102:GLN:HE21	3:B:102:GLN:HB2	1.59	0.42
2:A:755:VAL:CG1	2:A:756:LEU:N	2.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1272:THR:O	2:A:1276:ASN:HB2	2.19	0.42
2:A:1694:ILE:CG1	2:A:1703:LEU:CD1	2.97	0.42
3:B:101:LEU:O	3:B:102:GLN:CB	2.65	0.42
3:B:141:LYS:NZ	3:B:141:LYS:CB	2.73	0.42
1:C:59:ASN:HB3	1:C:62:GLN:CG	2.50	0.42
1:C:108:TYR:N	1:C:108:TYR:CD1	2.86	0.42
2:A:215:THR:HA	2:A:218:VAL:HG23	2.02	0.42
2:A:333:ILE:CG2	2:A:334:GLY:N	2.82	0.42
2:A:773:LYS:HA	2:A:773:LYS:HD2	1.63	0.42
2:A:731:ILE:HG12	2:A:734:LYS:HE3	2.01	0.42
2:A:1277:THR:CG2	2:A:1278:LEU:N	2.82	0.42
2:A:1389:PHE:HZ	2:A:1399:LEU:HD12	1.84	0.42
3:B:126:LEU:HD23	3:B:126:LEU:HA	1.88	0.42
2:A:278:ASN:N	2:A:278:ASN:HD22	2.16	0.42
2:A:800:PRO:O	2:A:804:PHE:HB2	2.20	0.42
2:A:849:TRP:HE3	2:A:852:LEU:HD23	1.84	0.42
2:A:1293:ARG:NH2	2:A:1293:ARG:CG	2.83	0.42
2:A:1487:LYS:HA	2:A:1487:LYS:HD3	1.58	0.42
2:A:1595:LEU:HD12	2:A:1595:LEU:HA	1.91	0.42
3:B:90:VAL:HG11	3:B:106:ILE:HD11	2.02	0.42
2:A:168:LEU:CD2	2:A:169:VAL:N	2.73	0.41
2:A:191:LEU:C	2:A:191:LEU:CD2	2.86	0.41
2:A:329:THR:CG2	2:A:330:CYS:N	2.82	0.41
2:A:1508:ILE:HG23	2:A:1564:LEU:CD1	2.50	0.41
2:A:254:PHE:O	2:A:258:VAL:HG23	2.20	0.41
2:A:736:CYS:C	2:A:740:ILE:HG12	2.40	0.41
2:A:737:ILE:O	2:A:741:VAL:N	2.51	0.41
2:A:803:TYR:CE1	2:A:809:ASN:ND2	2.88	0.41
2:A:1314:LEU:HA	2:A:1314:LEU:HD12	1.83	0.41
2:A:1499:ARG:HH11	2:A:1501:GLY:C	2.24	0.41
2:A:1552:VAL:O	2:A:1556:ILE:HG13	2.19	0.41
2:A:217:ARG:NH1	2:A:217:ARG:CG	2.82	0.41
2:A:278:ASN:ND2	2:A:278:ASN:N	2.69	0.41
2:A:371:LEU:HD11	2:A:379:MET:HA	2.02	0.41
2:A:1473:PHE:CE1	2:A:1753:ASN:ND2	2.88	0.41
3:B:174:LEU:HD13	3:B:178:MET:CG	2.49	0.41
2:A:791:MET:CE	2:A:795:LEU:HD11	2.51	0.41
2:A:818:LEU:HD12	2:A:818:LEU:HA	1.85	0.41
2:A:960:LEU:HD23	2:A:960:LEU:C	2.41	0.41
2:A:1268:VAL:HG12	2:A:1289:LEU:HD13	2.01	0.41
2:A:1450:ASN:C	2:A:1450:ASN:ND2	2.73	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1637:LEU:C	2:A:1637:LEU:CD2	2.89	0.41
3:B:62:LYS:HG3	3:B:63:GLY:N	2.35	0.41
2:A:224:THR:O	2:A:227:VAL:HG23	2.19	0.41
2:A:303:PHE:N	2:A:303:PHE:HD1	2.18	0.41
2:A:370:THR:OG1	2:A:382:PHE:CE2	2.73	0.41
2:A:1295:LEU:HD13	2:A:1295:LEU:HA	1.87	0.41
2:A:1350:CYS:SG	2:A:1382:TRP:CZ3	3.12	0.41
2:A:1358:ARG:CZ	2:A:1417:ASP:OD2	2.68	0.41
3:B:46:ARG:NH2	3:B:48:GLU:OE1	2.53	0.41
2:A:163:TYR:N	2:A:163:TYR:CD1	2.89	0.41
2:A:180:GLU:HB2	2:A:183:PHE:HB3	2.02	0.41
2:A:222:LEU:C	2:A:224:THR:N	2.73	0.41
2:A:406:LYS:HB2	2:A:406:LYS:HE2	1.78	0.41
2:A:765:HIS:CD2	2:A:768:MET:HG2	2.56	0.41
2:A:1340:VAL:O	2:A:1344:ALA:CB	2.68	0.41
2:A:1595:LEU:C	2:A:1599:ILE:HD12	2.36	0.41
3:B:59:PHE:CD2	3:B:119:TYR:CE1	3.08	0.41
2:A:147:ASN:ND2	2:A:147:ASN:O	2.54	0.41
2:A:153:LYS:O	2:A:157:TYR:CD2	2.74	0.41
2:A:175:GLY:CA	2:A:180:GLU:HA	2.50	0.41
2:A:188:TRP:CG	2:A:232:LYS:HE2	2.52	0.41
2:A:403:MET:O	2:A:403:MET:SD	2.79	0.41
3:B:50:ASN:C	3:B:50:ASN:HD22	2.24	0.41
1:C:32:VAL:CA	1:C:51:THR:O	2.64	0.41
2:A:388:LEU:C	2:A:388:LEU:CD1	2.85	0.41
2:A:393:LEU:HD23	2:A:393:LEU:HA	1.79	0.41
2:A:1457:ILE:CD1	2:A:1458:ASP:N	2.73	0.41
3:B:60:ARG:CB	3:B:66:GLU:O	2.69	0.41
3:B:89:ARG:HG3	3:B:89:ARG:NH1	2.22	0.41
2:A:200:TYR:N	2:A:200:TYR:HD1	2.18	0.41
2:A:361:ASP:OD2	2:A:929:ILE:HB	2.20	0.41
2:A:752:ILE:HD13	2:A:752:ILE:HA	1.90	0.41
2:A:766:HIS:CD2	2:A:766:HIS:O	2.73	0.41
2:A:779:GLY:O	2:A:783:PHE:HD2	2.03	0.41
2:A:791:MET:HE2	2:A:791:MET:HB3	1.92	0.41
2:A:803:TYR:CE1	2:A:809:ASN:OD1	2.74	0.41
2:A:1293:ARG:HD2	2:A:1296:ARG:HH21	1.82	0.41
2:A:1329:LEU:HD22	2:A:1396:TYR:CE1	2.55	0.41
2:A:1580:ILE:O	2:A:1584:VAL:HG23	2.21	0.41
2:A:1588:ILE:CG2	2:A:1615:ALA:HB1	2.42	0.41
2:A:1622:ARG:HE	2:A:1622:ARG:HB3	1.79	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1634:LEU:HD13	2:A:1634:LEU:HA	1.84	0.41
3:B:44:LYS:NZ	3:B:100:ASP:OD2	2.54	0.41
3:B:50:ASN:ND2	3:B:50:ASN:C	2.73	0.41
1:C:38:LEU:HD23	1:C:48:LEU:HD22	2.03	0.41
2:A:146:ASN:O	2:A:147:ASN:CB	2.69	0.41
2:A:811:PHE:CD1	2:A:811:PHE:O	2.74	0.41
2:A:1519:ILE:N	2:A:1519:ILE:HD12	2.36	0.41
2:A:1601:THR:C	2:A:1602:TYR:HD1	2.23	0.41
2:A:114:PRO:CG	2:A:115:LEU:N	2.85	0.40
2:A:234:ILE:HG13	2:A:868:ASN:HB3	2.03	0.40
2:A:838:ARG:O	2:A:841:ARG:CD	2.69	0.40
2:A:1283:LEU:HG	2:A:1283:LEU:O	2.21	0.40
2:A:1647:ILE:HG23	2:A:1750:VAL:HG13	2.02	0.40
2:A:1737:ILE:O	2:A:1741:VAL:HG23	2.21	0.40
2:A:1767:THR:HG23	2:A:1768:GLU:N	2.35	0.40
2:A:183:PHE:CZ	2:A:189:ASN:OD1	2.74	0.40
2:A:364:GLU:HG2	2:A:365:ASN:N	2.36	0.40
2:A:916:SER:O	2:A:920:VAL:HG23	2.22	0.40
2:A:1509:PHE:HA	2:A:1512:VAL:CG2	2.52	0.40
3:B:83:ASP:O	3:B:87:GLU:HB2	2.20	0.40
3:B:121:CYS:O	3:B:121:CYS:SG	2.79	0.40
2:A:133:MET:O	2:A:136:ILE:HG22	2.20	0.40
2:A:196:ILE:HD12	2:A:197:VAL:H	1.81	0.40
2:A:757:ASN:ND2	2:A:757:ASN:C	2.73	0.40
2:A:808:TRP:O	2:A:811:PHE:HB3	2.22	0.40
2:A:1194:PHE:CD1	2:A:1194:PHE:C	2.94	0.40
1:C:107:LYS:O	1:C:108:TYR:CB	2.70	0.40
2:A:176:PHE:CD2	2:A:178:VAL:CG2	3.05	0.40
2:A:271:LEU:O	2:A:314:LEU:HD11	2.20	0.40
2:A:363:TRP:CZ3	2:A:367:TYR:CG	3.08	0.40
2:A:379:MET:HE2	2:A:379:MET:HB3	1.88	0.40
2:A:905:LEU:HD12	2:A:905:LEU:HA	1.95	0.40
2:A:952:MET:O	2:A:956:ASN:HB2	2.20	0.40
2:A:971:PHE:CD1	2:A:972:SER:HB2	2.56	0.40
2:A:1286:ILE:HA	2:A:1286:ILE:HD12	1.77	0.40
3:B:46:ARG:NH2	3:B:48:GLU:CD	2.73	0.40
2:A:338:ASP:O	2:A:339:TYR:CB	2.70	0.40
2:A:1254:PHE:HD1	2:A:1260:TRP:NE1	2.20	0.40
2:A:1273:LEU:O	2:A:1277:THR:CB	2.65	0.40
2:A:1459:ASN:ND2	2:A:1459:ASN:C	2.73	0.40
2:A:1680:ASN:OD1	2:A:1686:ASN:ND2	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:37:LYS:HB2	3:B:107:PHE:CD1	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	118/215 (55%)	110 (93%)	5 (4%)	3 (2%)	5 32
2	A	1132/2031 (56%)	1090 (96%)	27 (2%)	15 (1%)	12 47
3	B	171/218 (78%)	167 (98%)	3 (2%)	1 (1%)	25 64
All	All	1421/2464 (58%)	1367 (96%)	35 (2%)	19 (1%)	16 47

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	147	ASN
2	A	743	ASP
2	A	836	SER
2	A	896	VAL
2	A	1282	ASP
2	A	305	TYR
2	A	897	CYS
2	A	899	ILE
2	A	1617	ILE
1	C	56	TYR
1	C	76	SER
2	A	767	PRO
2	A	1386	LYS
2	A	1497	ILE
1	C	147	LEU
3	B	66	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	842	VAL
2	A	1498	PRO
2	A	1711	LYS

5.3.2 Protein sidechains (i)

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	C	113/193 (58%)	101 (89%)	12 (11%)	6 27
2	A	1018/1809 (56%)	746 (73%)	272 (27%)	0 2
3	B	157/190 (83%)	105 (67%)	52 (33%)	0 0
All	All	1288/2192 (59%)	952 (74%)	336 (26%)	2 2

All (336) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	30	MET
1	C	51	THR
1	C	52	PHE
1	C	59	ASN
1	C	61	LYS
1	C	74	ASN
1	C	107	LYS
1	C	129	ILE
1	C	134	ASP
1	C	135	ARG
1	C	147	LEU
1	C	148	MET
2	A	115	LEU
2	A	117	ARG
2	A	118	ILE
2	A	121	LYS
2	A	122	ILE
2	A	124	VAL
2	A	126	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	127	LEU
2	A	130	MET
2	A	131	LEU
2	A	134	CYS
2	A	136	ILE
2	A	137	LEU
2	A	138	THR
2	A	139	ASN
2	A	143	MET
2	A	145	MET
2	A	146	ASN
2	A	147	ASN
2	A	153	LYS
2	A	156	GLU
2	A	158	THR
2	A	166	GLU
2	A	167	SER
2	A	168	LEU
2	A	170	LYS
2	A	171	ILE
2	A	181	PHE
2	A	184	LEU
2	A	189	ASN
2	A	204	PHE
2	A	206	ASN
2	A	213	LEU
2	A	217	ARG
2	A	222	LEU
2	A	224	THR
2	A	227	VAL
2	A	232	LYS
2	A	238	LEU
2	A	240	GLN
2	A	245	LEU
2	A	249	MET
2	A	255	CYS
2	A	265	GLN
2	A	268	MET
2	A	271	LEU
2	A	277	ARG
2	A	280	LEU
2	A	291	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	293	LEU
2	A	294	GLU
2	A	295	SER
2	A	297	GLU
2	A	299	PHE
2	A	300	ARG
2	A	301	LYS
2	A	303	PHE
2	A	311	ASP
2	A	313	LEU
2	A	314	LEU
2	A	318	SER
2	A	348	SER
2	A	349	TRP
2	A	354	LEU
2	A	356	ARG
2	A	358	MET
2	A	362	TYR
2	A	364	GLU
2	A	366	LEU
2	A	367	TYR
2	A	370	THR
2	A	371	LEU
2	A	379	MET
2	A	387	PHE
2	A	403	MET
2	A	408	GLN
2	A	410	GLN
2	A	412	ASN
2	A	414	GLU
2	A	415	GLU
2	A	727	SER
2	A	732	LYS
2	A	733	PHE
2	A	735	LYS
2	A	738	TYR
2	A	739	PHE
2	A	748	LEU
2	A	751	THR
2	A	761	MET
2	A	763	MET
2	A	765	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	766	HIS
2	A	769	THR
2	A	772	PHE
2	A	773	LYS
2	A	791	MET
2	A	793	LEU
2	A	794	LYS
2	A	795	LEU
2	A	798	MET
2	A	804	PHE
2	A	805	GLN
2	A	808	TRP
2	A	811	PHE
2	A	813	SER
2	A	816	VAL
2	A	818	LEU
2	A	819	SER
2	A	820	LEU
2	A	822	GLU
2	A	823	LEU
2	A	831	LEU
2	A	832	SER
2	A	834	LEU
2	A	835	ARG
2	A	837	PHE
2	A	841	ARG
2	A	847	LYS
2	A	848	SER
2	A	852	LEU
2	A	857	LYS
2	A	862	SER
2	A	869	LEU
2	A	870	THR
2	A	871	LEU
2	A	873	LEU
2	A	887	LEU
2	A	890	LYS
2	A	898	LYS
2	A	900	ASN
2	A	901	ASP
2	A	902	ASP
2	A	905	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	910	MET
2	A	911	ASN
2	A	916	SER
2	A	918	LEU
2	A	922	ARG
2	A	929	ILE
2	A	934	ASP
2	A	941	GLN
2	A	943	MET
2	A	945	LEU
2	A	952	MET
2	A	956	ASN
2	A	962	LEU
2	A	964	LEU
2	A	966	LEU
2	A	967	LEU
2	A	968	LEU
2	A	1176	LYS
2	A	1187	LYS
2	A	1189	VAL
2	A	1191	HIS
2	A	1204	LEU
2	A	1206	SER
2	A	1209	LEU
2	A	1219	LYS
2	A	1223	LYS
2	A	1226	LEU
2	A	1230	ASP
2	A	1246	ILE
2	A	1251	LYS
2	A	1264	LEU
2	A	1265	ILE
2	A	1269	SER
2	A	1270	LEU
2	A	1274	VAL
2	A	1277	THR
2	A	1282	ASP
2	A	1287	LYS
2	A	1289	LEU
2	A	1290	ARG
2	A	1292	LEU
2	A	1293	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	1295	LEU
2	A	1298	LEU
2	A	1301	LEU
2	A	1305	GLU
2	A	1309	VAL
2	A	1314	LEU
2	A	1325	LEU
2	A	1326	LEU
2	A	1331	PHE
2	A	1342	LEU
2	A	1354	THR
2	A	1358	ARG
2	A	1385	LEU
2	A	1396	TYR
2	A	1404	THR
2	A	1406	LYS
2	A	1408	TRP
2	A	1409	THR
2	A	1410	ILE
2	A	1419	VAL
2	A	1422	ASP
2	A	1423	LYS
2	A	1424	GLN
2	A	1426	LYS
2	A	1431	LEU
2	A	1449	LEU
2	A	1450	ASN
2	A	1452	PHE
2	A	1459	ASN
2	A	1461	ASN
2	A	1462	GLN
2	A	1464	LYS
2	A	1465	LYS
2	A	1467	LEU
2	A	1470	GLN
2	A	1478	GLN
2	A	1479	LYS
2	A	1486	LYS
2	A	1488	LEU
2	A	1491	LYS
2	A	1495	LYS
2	A	1499	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	1504	ILE
2	A	1505	GLN
2	A	1507	CYS
2	A	1512	VAL
2	A	1518	ASP
2	A	1519	ILE
2	A	1520	SER
2	A	1522	MET
2	A	1527	LEU
2	A	1528	ASN
2	A	1532	MET
2	A	1533	MET
2	A	1534	VAL
2	A	1537	GLU
2	A	1540	SER
2	A	1543	MET
2	A	1544	THR
2	A	1548	TYR
2	A	1551	ASN
2	A	1557	LEU
2	A	1561	GLU
2	A	1562	CYS
2	A	1565	LYS
2	A	1571	HIS
2	A	1573	TYR
2	A	1593	MET
2	A	1595	LEU
2	A	1600	GLU
2	A	1601	THR
2	A	1603	PHE
2	A	1605	SER
2	A	1608	LEU
2	A	1616	ARG
2	A	1619	ARG
2	A	1628	LYS
2	A	1630	ILE
2	A	1634	LEU
2	A	1637	LEU
2	A	1644	LEU
2	A	1649	LEU
2	A	1653	LEU
2	A	1661	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	1670	LYS
2	A	1671	LYS
2	A	1673	ASP
2	A	1677	ASP
2	A	1683	THR
2	A	1687	SER
2	A	1691	LEU
2	A	1694	ILE
2	A	1704	LEU
2	A	1711	LYS
2	A	1718	LYS
2	A	1735	VAL
2	A	1749	LEU
3	B	27	GLU
3	B	28	THR
3	B	32	TYR
3	B	34	MET
3	B	39	LEU
3	B	43	CYS
3	B	46	ARG
3	B	47	SER
3	B	48	GLU
3	B	50	ASN
3	B	60	ARG
3	B	62	LYS
3	B	65	GLU
3	B	66	GLU
3	B	75	ASN
3	B	78	LEU
3	B	81	GLU
3	B	84	GLU
3	B	85	ARG
3	B	87	GLU
3	B	89	ARG
3	B	90	VAL
3	B	99	LYS
3	B	101	LEU
3	B	102	GLN
3	B	104	LEU
3	B	109	THR
3	B	121	CYS
3	B	125	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	126	LEU
3	B	127	LEU
3	B	130	GLU
3	B	131	ASN
3	B	136	THR
3	B	138	VAL
3	B	141	LYS
3	B	142	ILE
3	B	144	ILE
3	B	149	LYS
3	B	151	ASN
3	B	152	ARG
3	B	153	ASP
3	B	157	ILE
3	B	162	MET
3	B	166	LEU
3	B	174	LEU
3	B	177	GLU
3	B	178	MET
3	B	183	LYS
3	B	184	LYS
3	B	190	GLU
3	B	191	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	82	GLN
1	C	118	GLN
2	A	147	ASN
2	A	154	ASN
2	A	189	ASN
2	A	278	ASN
2	A	282	ASN
2	A	291	ASN
2	A	360	GLN
2	A	365	ASN
2	A	410	GLN
2	A	412	ASN
2	A	766	HIS
2	A	774	ASN
2	A	909	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	956	ASN
2	A	1424	GLN
2	A	1450	ASN
2	A	1505	GLN
2	A	1514	ASN
2	A	1528	ASN
2	A	1571	HIS
2	A	1721	HIS
2	A	1753	ASN
2	A	1762	ASN
3	B	50	ASN
3	B	75	ASN
3	B	102	GLN
3	B	134	HIS
3	B	151	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

4 monosaccharides 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	$\#\|Z\| > 2$
4	NAG	D	1	2,4	14,14,15	0.45	0	17,19,21	0.98	1 (5%)
4	NAG	D	2	4	14,14,15	0.39	0	17,19,21	1.31	2 (11%)
4	NAG	E	1	2,4	14,14,15	0.38	0	17,19,21	1.08	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	E	2	4	14,14,15	0.42	0	17,19,21	1.19	2 (11%)

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
4	NAG	D	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	4/6/23/26	0/1/1/1
4	NAG	E	1	2,4	-	6/6/23/26	0/1/1/1
4	NAG	E	2	4	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1	NAG	O5-C1-C2	-3.10	106.39	111.29
4	E	2	NAG	C1-O5-C5	-3.07	108.03	112.19
4	D	2	NAG	C1-O5-C5	2.71	115.86	112.19
4	E	2	NAG	O5-C5-C6	2.64	111.35	107.20
4	D	2	NAG	C2-N2-C7	-2.62	119.17	122.90
4	E	1	NAG	O4-C4-C3	-2.17	105.32	110.35
4	D	1	NAG	O5-C5-C6	2.15	110.58	107.20

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
4	D	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	E	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C1-C2-N2-C7
4	E	2	NAG	C3-C2-N2-C7
4	E	1	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

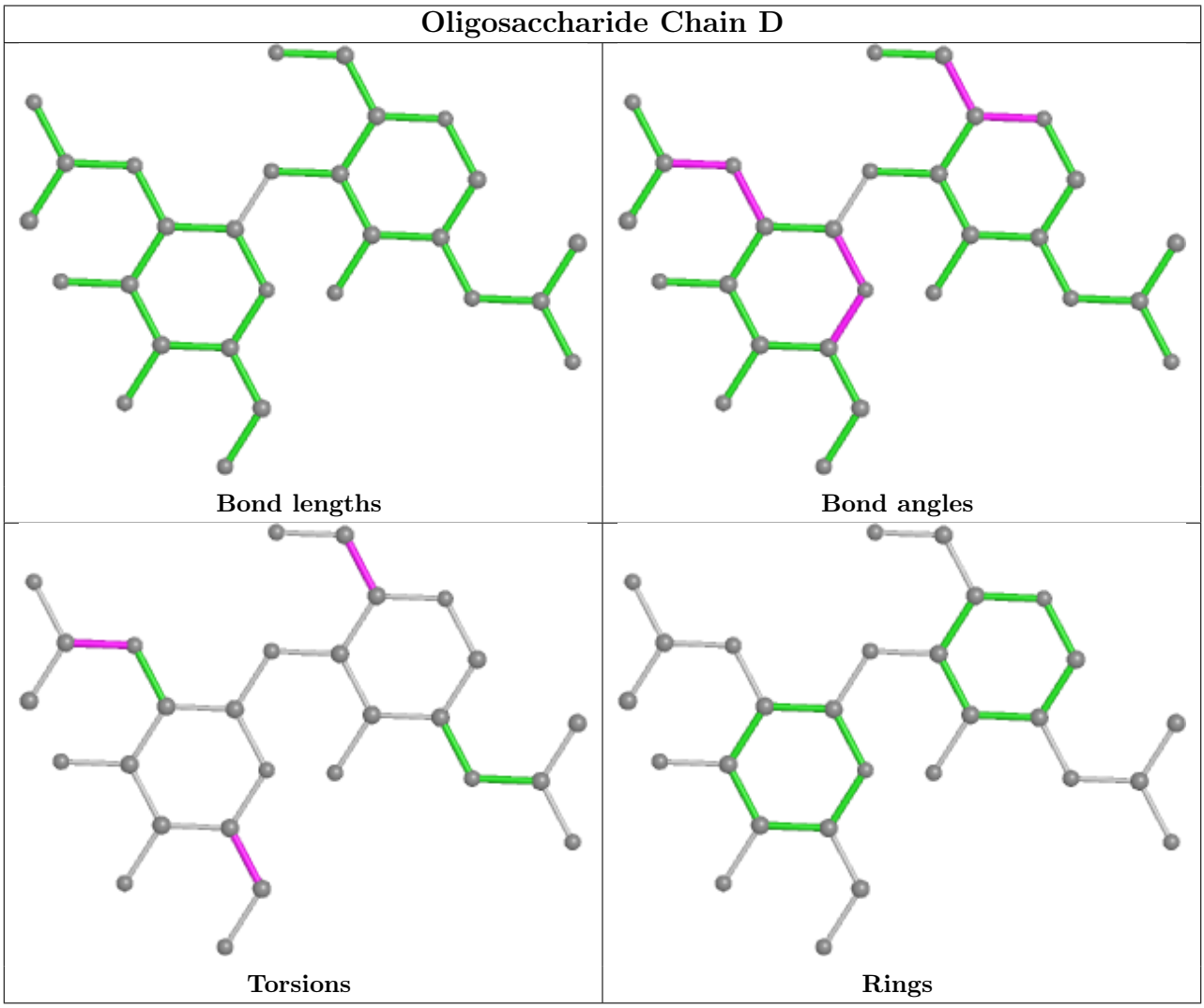
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C4-C5-C6-O6
4	E	1	NAG	C1-C2-N2-C7
4	D	1	NAG	C4-C5-C6-O6
4	E	1	NAG	C3-C2-N2-C7
4	D	1	NAG	O5-C5-C6-O6

There are no ring outliers.

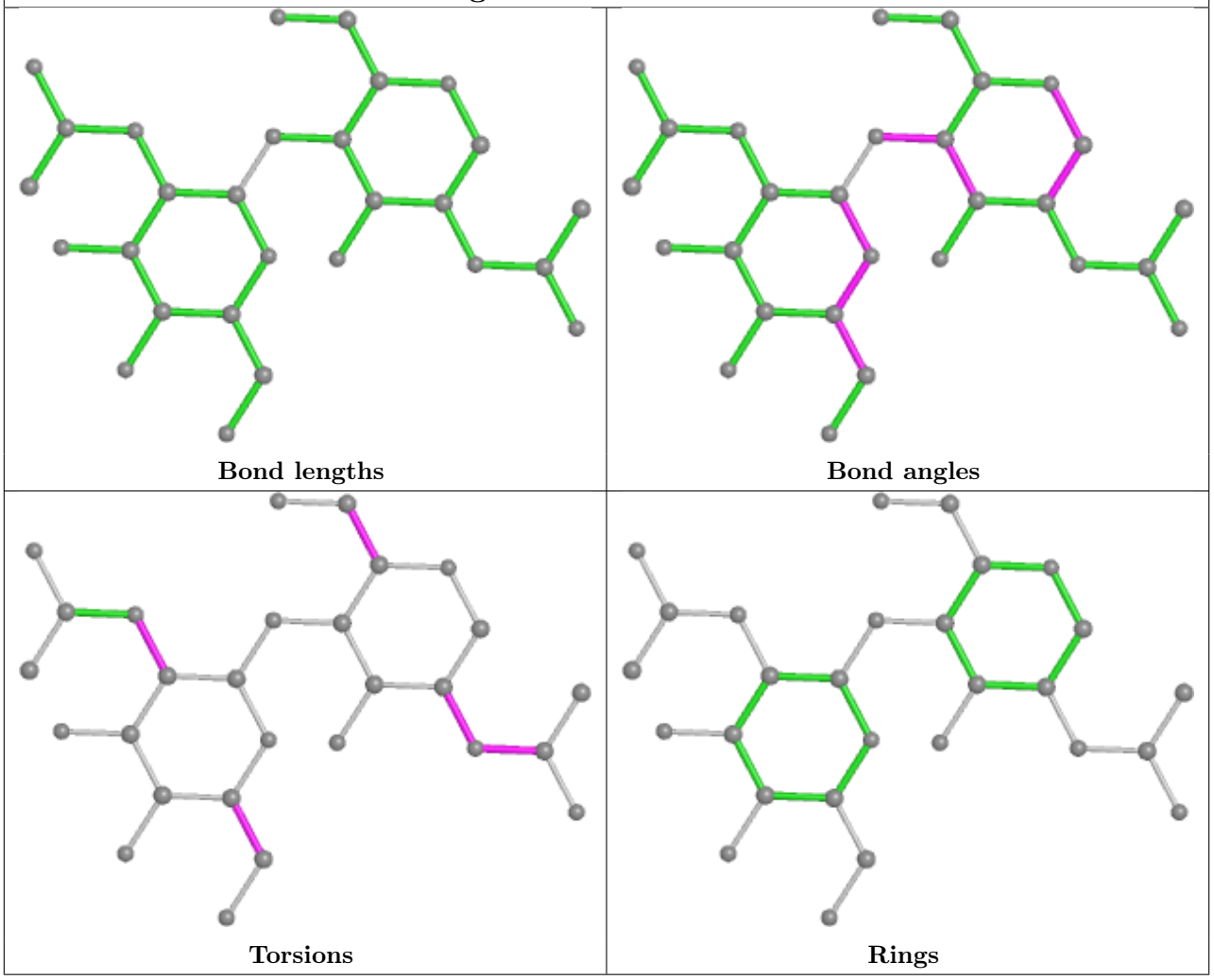
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	2	NAG	2	0
4	E	1	NAG	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



Oligosaccharide Chain E



5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
5	NAG	C	301	1	14,14,15	0.35	0	17,19,21	0.37	0
5	NAG	B	301	3	14,14,15	0.35	0	17,19,21	0.35	0
5	NAG	B	302	3	14,14,15	0.34	0	17,19,21	0.46	0
5	NAG	B	304	3	14,14,15	0.36	0	17,19,21	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	B	303	3	14,14,15	0.35	0	17,19,21	0.49	0
5	NAG	A	2006	2	14,14,15	0.36	0	17,19,21	0.37	0
6	9SR	A	2007	-	16,25,25	2.72	6 (37%)	18,44,44	1.74	2 (11%)
5	NAG	A	2005	2	14,14,15	0.36	0	17,19,21	0.37	0

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
5	NAG	C	301	1	-	2/6/23/26	0/1/1/1
5	NAG	B	301	3	-	2/6/23/26	0/1/1/1
5	NAG	B	302	3	-	2/6/23/26	0/1/1/1
5	NAG	B	304	3	-	2/6/23/26	0/1/1/1
5	NAG	B	303	3	-	2/6/23/26	0/1/1/1
5	NAG	A	2006	2	-	2/6/23/26	0/1/1/1
6	9SR	A	2007	-	-	0/3/70/70	0/5/4/4
5	NAG	A	2005	2	-	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2007	9SR	C21-C03	5.11	1.63	1.52
6	A	2007	9SR	C13-N18	4.56	1.45	1.34
6	A	2007	9SR	C03-C05	-4.26	1.45	1.53
6	A	2007	9SR	C03-C02	-4.08	1.45	1.53
6	A	2007	9SR	O20-C19	-3.72	1.35	1.42
6	A	2007	9SR	O04-C03	-2.78	1.39	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	2007	9SR	C17-C11-N12	5.64	114.34	108.12
6	A	2007	9SR	C03-C02-C19	-2.60	110.31	114.38

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	301	NAG	O5-C5-C6-O6
5	A	2005	NAG	O5-C5-C6-O6
5	A	2006	NAG	O5-C5-C6-O6
5	B	301	NAG	O5-C5-C6-O6
5	B	303	NAG	O5-C5-C6-O6
5	B	304	NAG	O5-C5-C6-O6
5	C	301	NAG	C4-C5-C6-O6
5	A	2005	NAG	C4-C5-C6-O6
5	A	2006	NAG	C4-C5-C6-O6
5	B	301	NAG	C4-C5-C6-O6
5	B	304	NAG	C4-C5-C6-O6
5	B	303	NAG	C4-C5-C6-O6
5	B	302	NAG	C4-C5-C6-O6
5	B	302	NAG	O5-C5-C6-O6

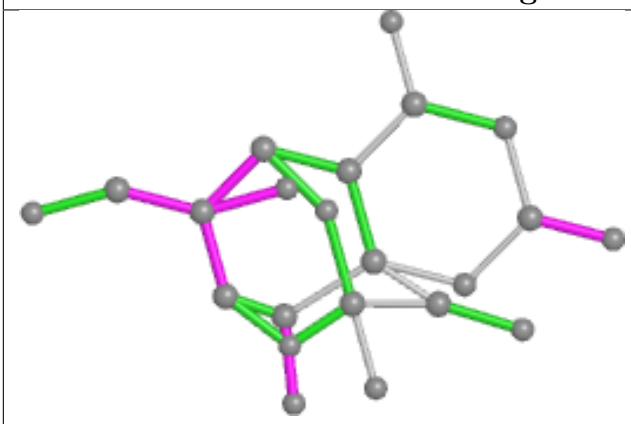
There are no ring outliers.

4 monomers are involved in 18 short contacts:

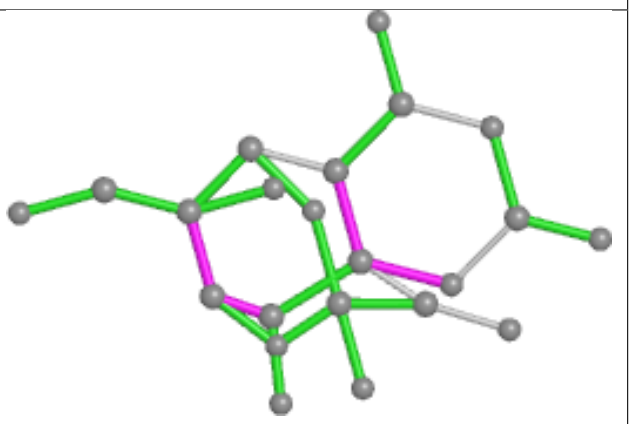
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	301	NAG	15	0
5	B	303	NAG	1	0
5	A	2006	NAG	1	0
6	A	2007	9SR	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

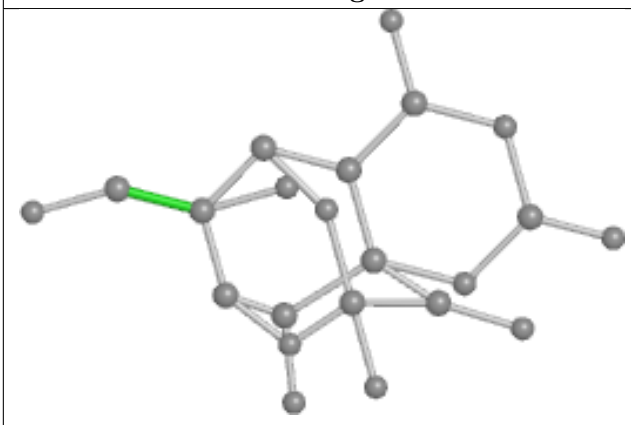
Ligand 9SR A 2007



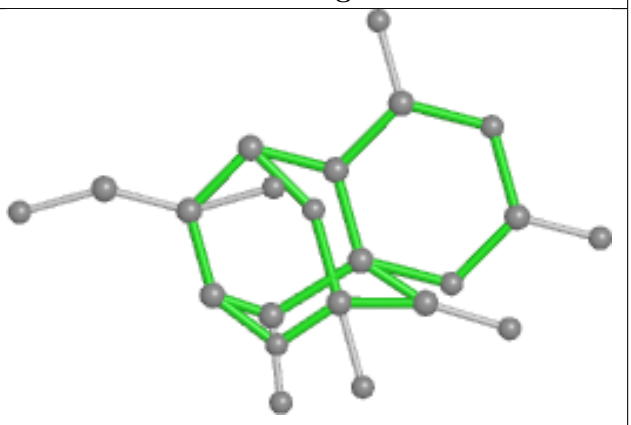
Bond lengths



Bond angles



Torsions



Rings

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.

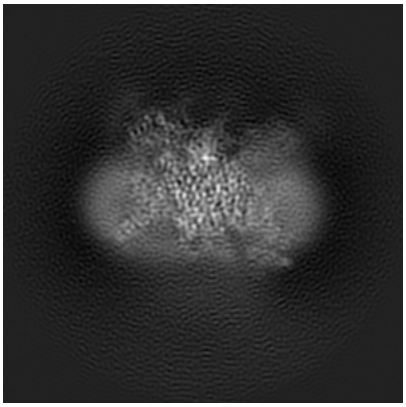
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9782. These allow visual inspection of the internal detail of the map and identification of artifacts.

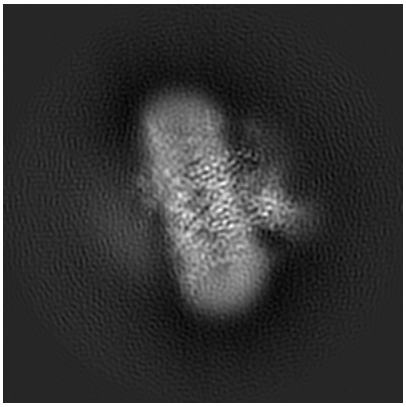
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

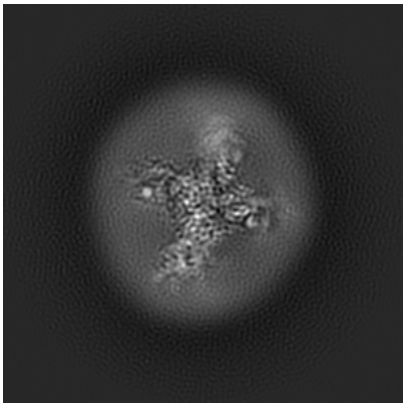
6.1.1 Primary map



X



Y

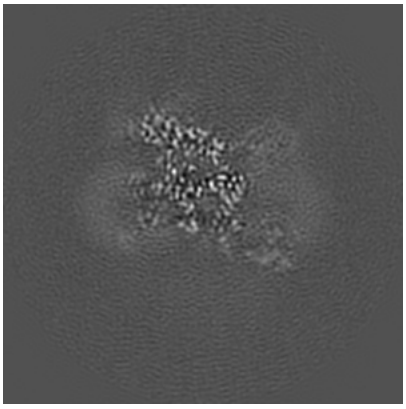


Z

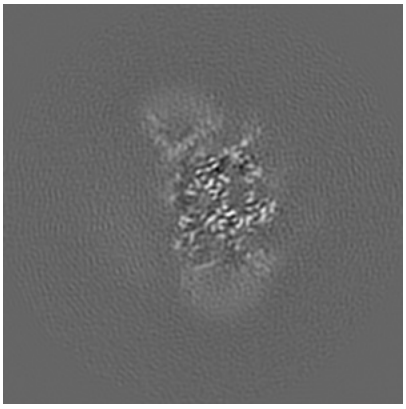
The images above show the map projected in three orthogonal directions.

6.2 Central slices

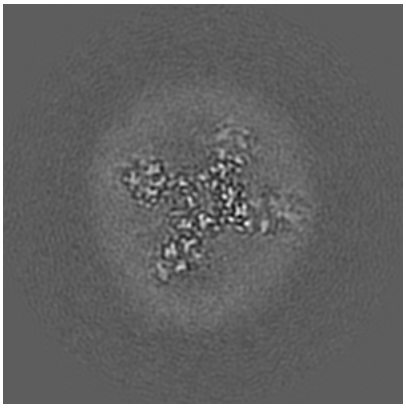
6.2.1 Primary map



X Index: 120



Y Index: 120

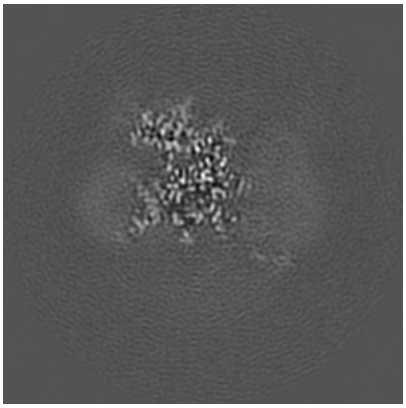


Z Index: 120

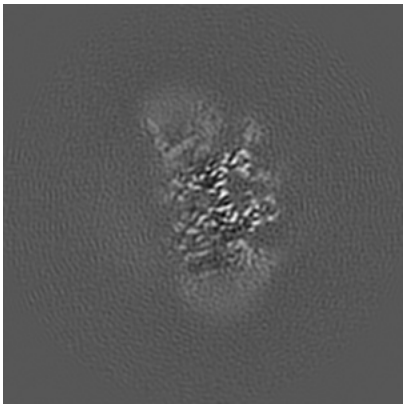
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

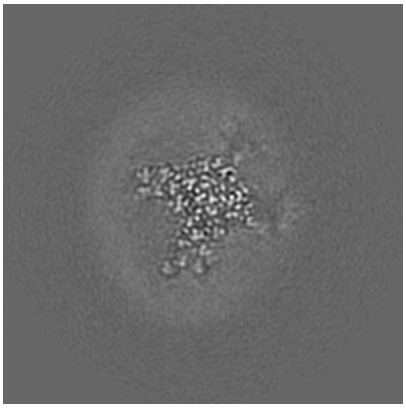
6.3.1 Primary map



X Index: 114



Y Index: 122



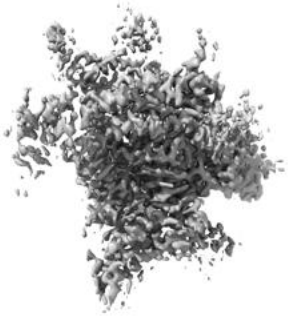
Z Index: 131

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

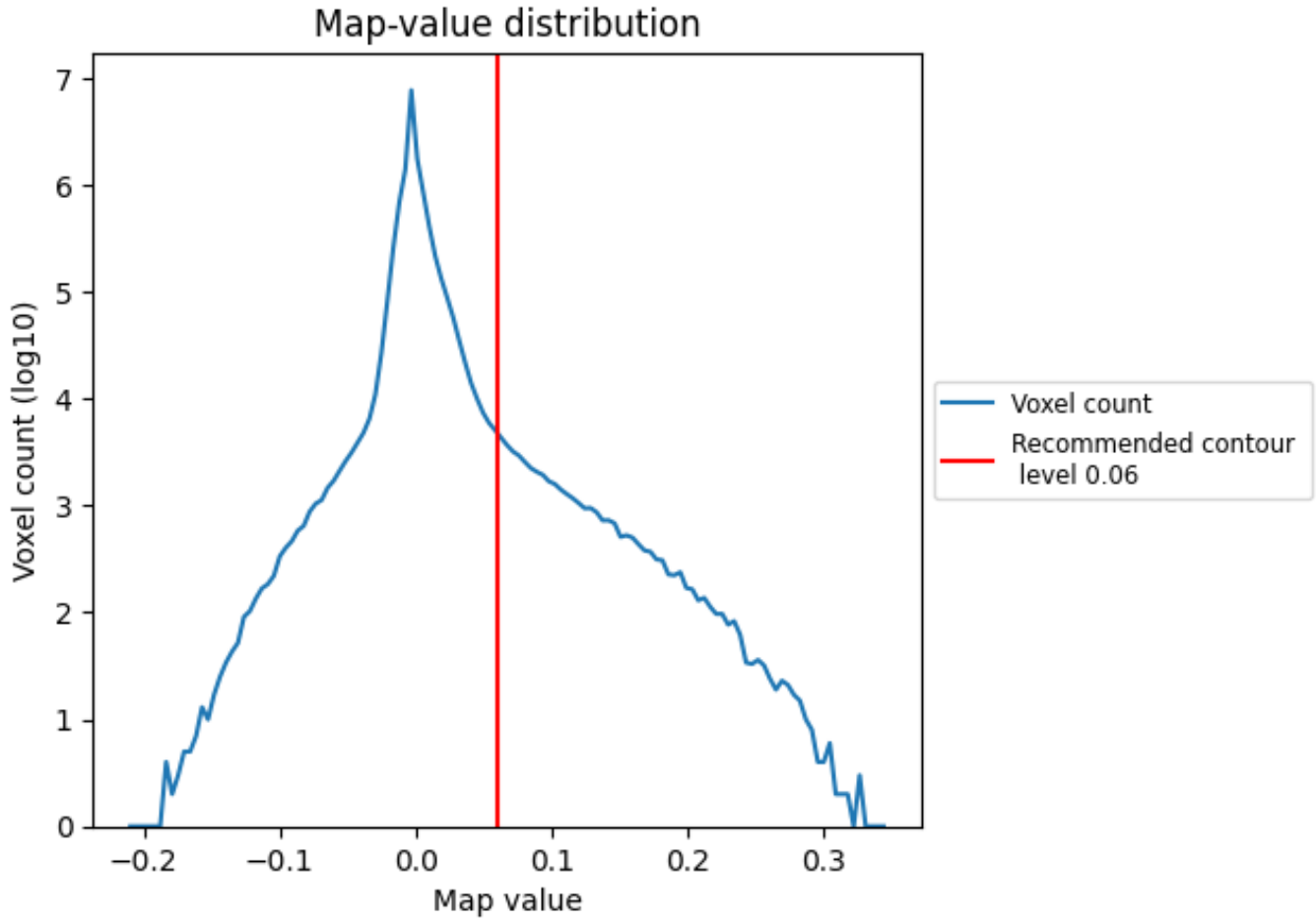
6.5 Mask visualisation (i)

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

7 Map analysis

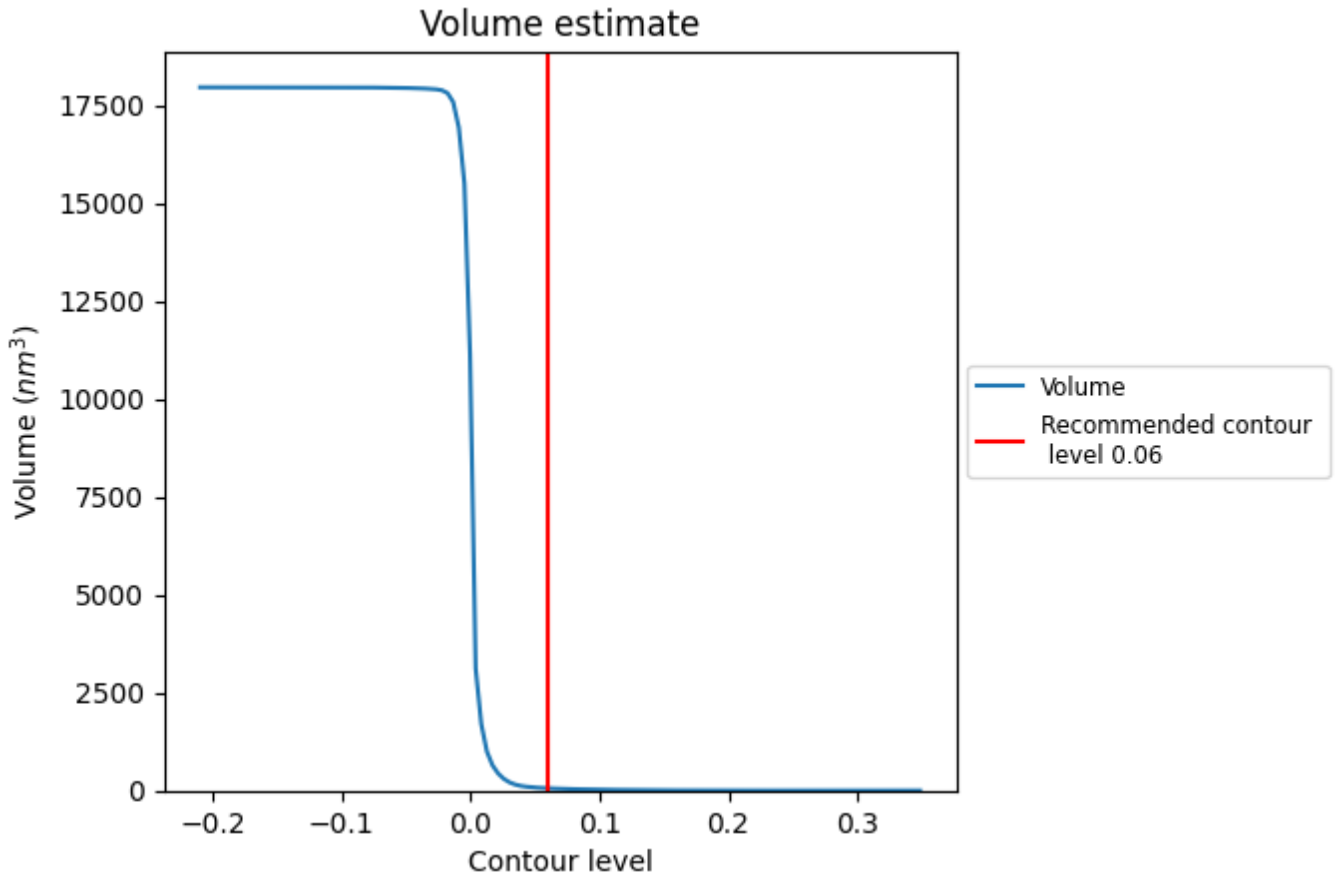
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

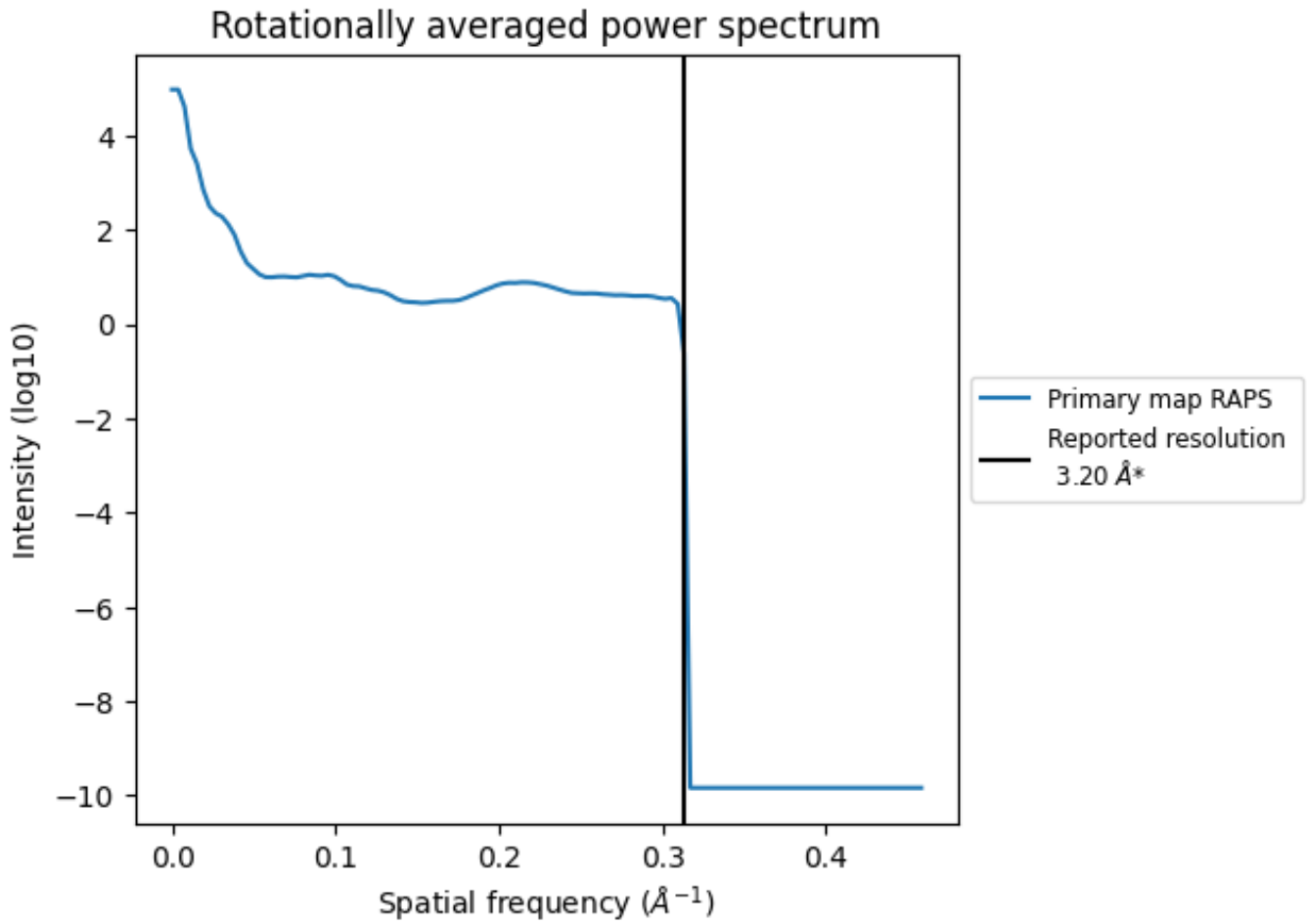
7.2 Volume estimate (i)



The volume at the recommended contour level is 58 nm^3; this corresponds to an approximate mass of 52 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 (i)



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

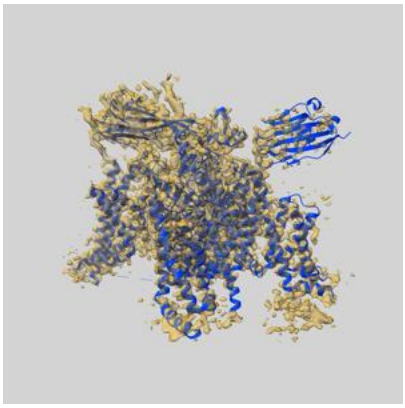
8 Fourier-Shell correlation

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

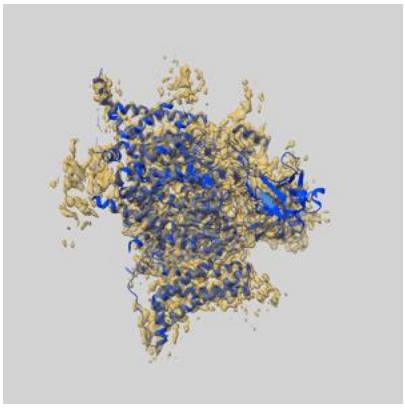
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9782 and PDB model 6J8I. Per-residue inclusion information can be found in section 3 on page 8.

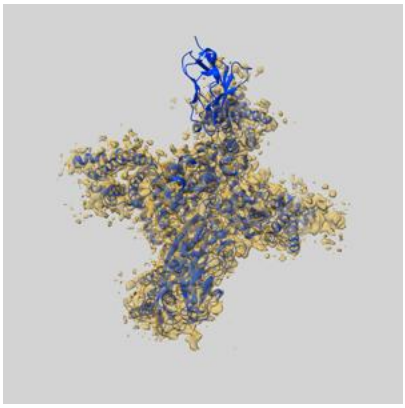
9.1 Map-model overlay



X



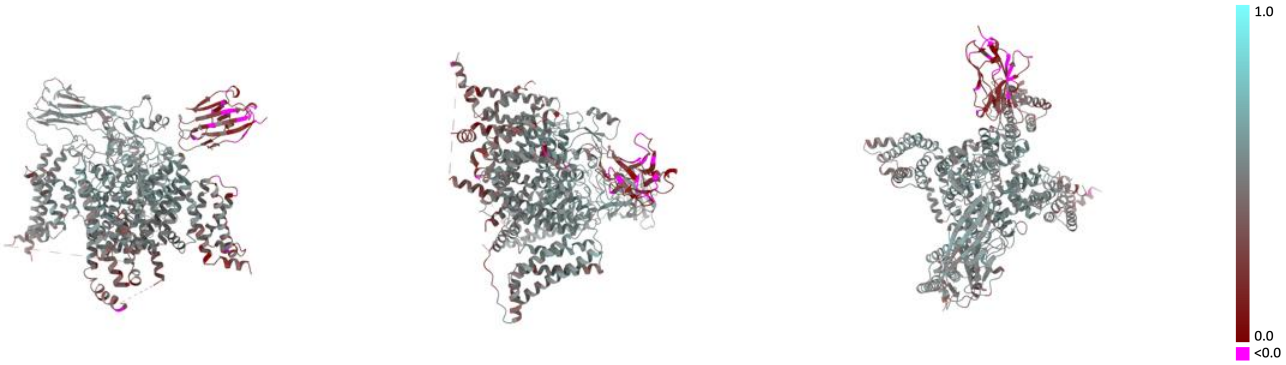
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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.

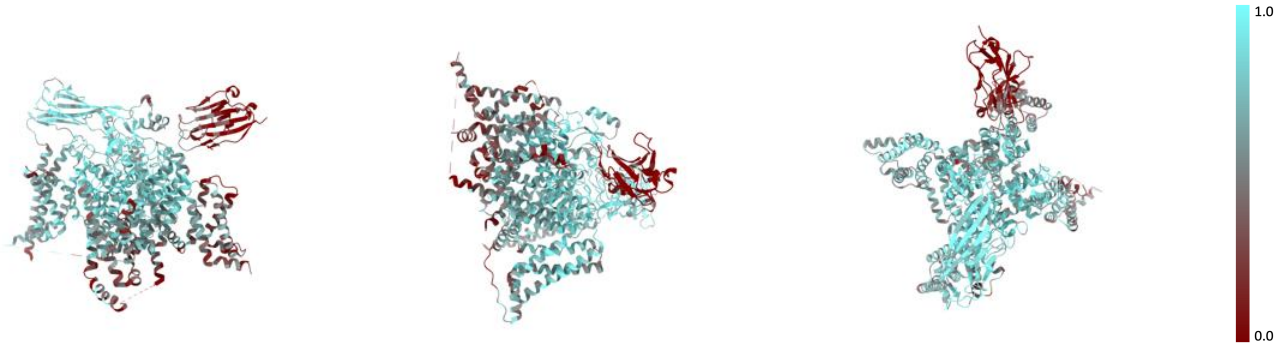
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

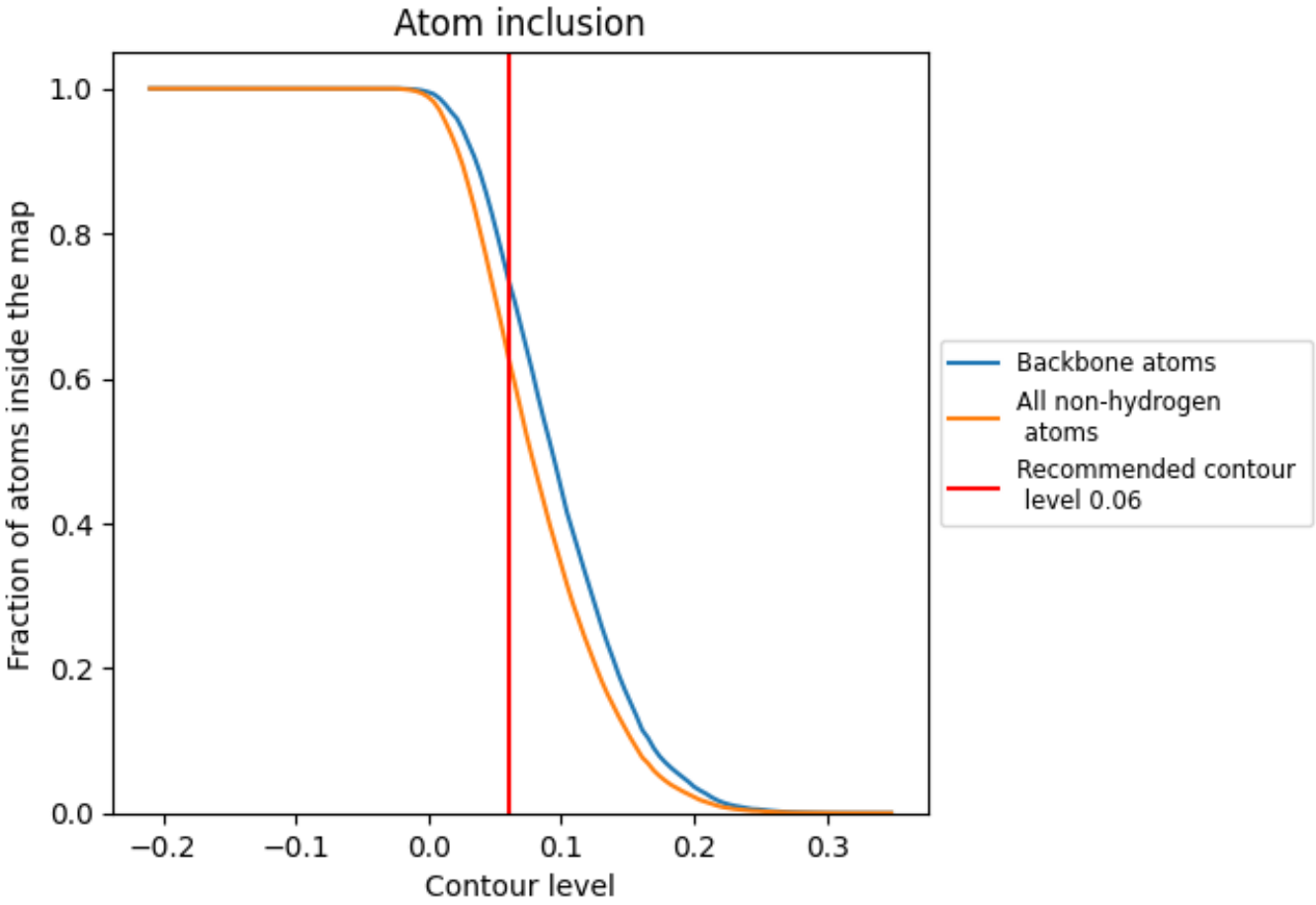
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 63% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6300	0.4600
A	0.6721	0.4860
B	0.7122	0.4870
C	0.1201	0.1790
D	0.5000	0.4440
E	0.5714	0.3340