



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:30 PM UTC

PDB ID : 6J8G / pdb_00006j8g
EMDB ID : EMD-9781
Title : Structure of human voltage-gated sodium channel Nav1.7 in complex with auxiliary beta subunits, huwentoxin-IV and saxitoxin (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:

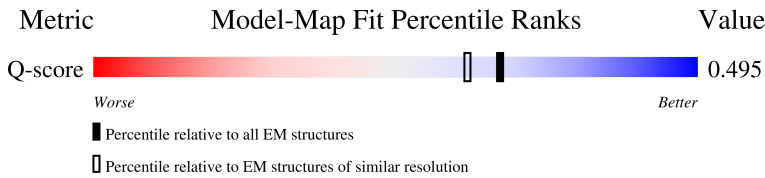
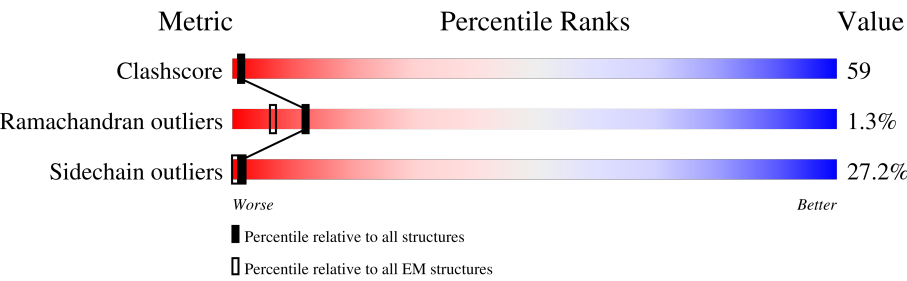
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	215	52% 29% 20% 7% 44%
2	A	2031	7% 19% 25% 11% 44%
3	B	218	6% 24% 37% 17% 21%
4	D	2	50% 50% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	2	 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11763 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.



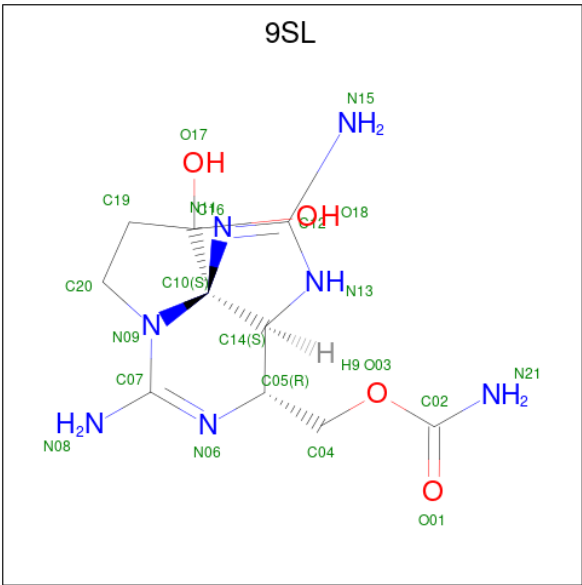
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

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



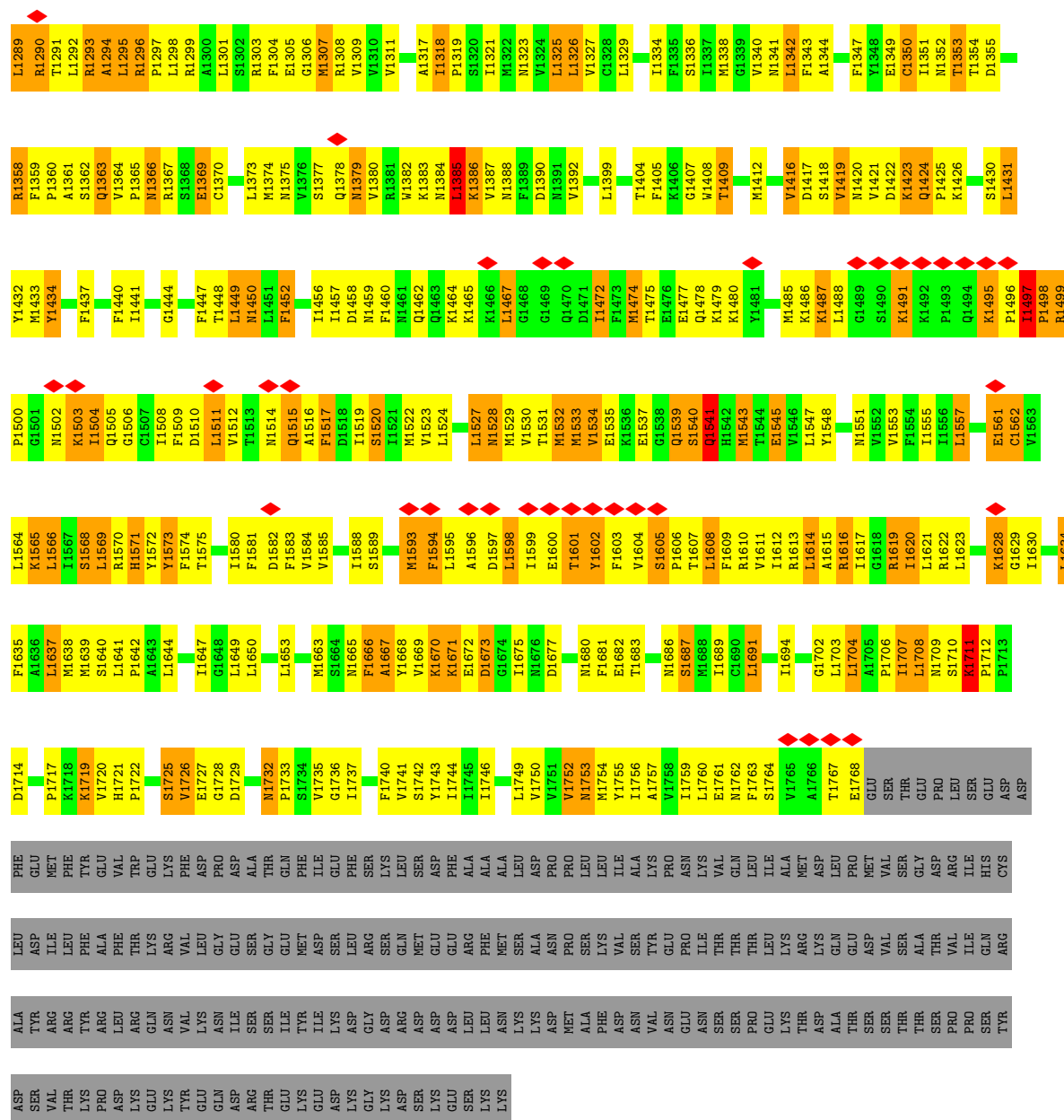
Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 6 is [(3aS,4R,10aS)-2,6-diamino-10,10-dihydroxy-3a,4,9,10-tetrahydro-3H,8H-pyrrolo[1,2-c]purin-4-yl]methyl carbamate (CCD ID: 9SL) (formula: $C_{10}H_{17}N_7O_4$).

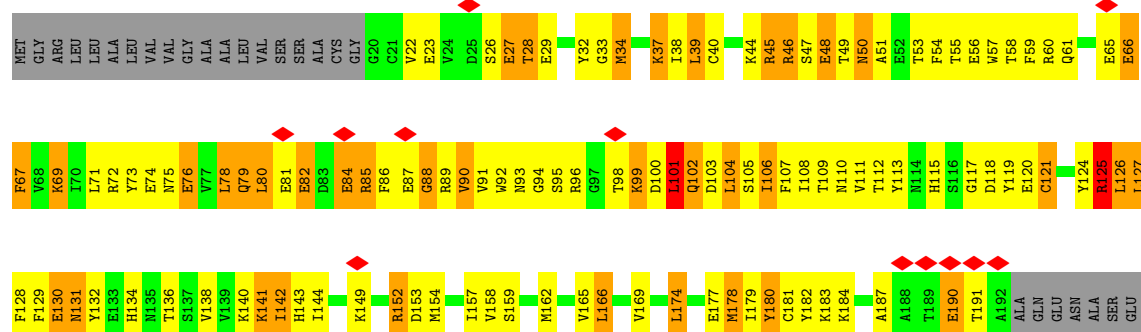
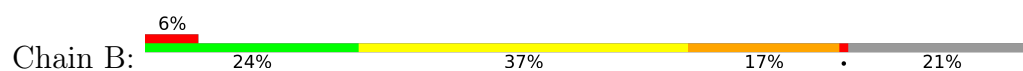


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	A	1	21	10	7	4	0





• Molecule 3: Sodium channel subunit beta-1



LEU	ALA	ILE	THR	SER	GLU	SER	LYS	GLU	ASN	CYS	THR	GLY	VAL	GLN	VAL	ALA	GLU
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	275630	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	0.410	Depositor
Minimum map value	-0.249	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.07	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, 9SL

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	0.44	1/1002 (0.1%)	0.83	5/1354 (0.4%)
2	A	0.74	1/9417 (0.0%)	1.12	86/12761 (0.7%)
3	B	0.64	0/1442	0.98	3/1949 (0.2%)
All	All	0.70	2/11861 (0.0%)	1.08	94/16064 (0.6%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	127	CYS	CB-SG	6.07	2.01	1.81
2	A	324	CYS	C-N	5.30	1.40	1.33

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	302	TYR	N-CA-C	12.27	124.73	111.36
2	A	925	CYS	N-CA-C	-11.99	94.36	110.55
2	A	304	TYR	N-CA-C	11.80	123.84	110.97
2	A	1378	GLN	N-CA-C	11.68	124.09	111.36
3	B	101	LEU	N-CA-C	10.23	122.02	111.07
2	A	929	ILE	N-CA-C	9.26	120.07	110.62
2	A	928	TRP	N-CA-C	8.90	120.98	111.28
2	A	1385	LEU	N-CA-C	8.80	120.87	111.28
2	A	941	GLN	N-CA-C	8.62	120.75	111.36
2	A	1720	VAL	N-CA-C	8.19	118.97	110.62
2	A	911	ASN	N-CA-C	8.07	120.08	111.28
2	A	1569	LEU	N-CA-C	8.07	120.16	111.36
2	A	1421	VAL	N-CA-C	8.06	118.84	110.62
2	A	227	VAL	N-CA-C	7.99	118.08	110.42
2	A	1712	PRO	C-N-CD	7.77	137.69	120.60
1	C	131	ASN	CA-C-N	-7.72	114.10	119.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	131	ASN	C-N-CA	-7.72	114.10	119.66
2	A	1665	ASN	N-CA-C	7.66	119.42	111.14
2	A	1667	ALA	N-CA-C	-7.56	99.84	110.50
2	A	938	VAL	N-CA-C	7.51	117.59	110.53
2	A	345	ASP	N-CA-C	7.50	119.46	111.28
2	A	1539	GLN	N-CA-C	7.34	119.28	111.28
2	A	278	ASN	N-CA-C	7.29	119.22	111.28
2	A	1279	GLY	N-CA-C	-7.25	99.77	112.53
2	A	1711	LYS	CA-C-N	-7.16	114.50	119.66
2	A	1711	LYS	C-N-CA	-7.16	114.50	119.66
2	A	1218	ARG	N-CA-C	-7.14	100.91	110.55
2	A	1383	LYS	N-CA-C	7.13	120.28	109.23
2	A	837	PHE	N-CA-C	6.97	120.88	112.38
2	A	1541	GLN	N-CA-C	6.97	118.87	111.28
2	A	1666	PHE	N-CA-C	6.90	121.87	113.17
2	A	292	THR	N-CA-C	6.86	118.76	111.28
2	A	797	ALA	N-CA-C	6.82	118.71	111.28
2	A	307	GLU	N-CA-C	6.69	120.47	111.24
2	A	1379	ASN	N-CA-C	6.63	121.02	112.26
2	A	1362	SER	N-CA-C	-6.62	104.15	111.36
2	A	1387	VAL	N-CA-C	-6.47	98.19	107.77
3	B	88	GLY	N-CA-C	-6.32	101.20	112.58
2	A	208	GLY	N-CA-C	6.30	120.29	112.73
2	A	183	PHE	N-CA-C	6.24	117.88	111.14
2	A	1285	PRO	N-CA-C	-6.24	101.38	110.80
2	A	1284	GLY	CA-C-N	-6.20	113.39	119.90
2	A	1284	GLY	C-N-CA	-6.20	113.39	119.90
2	A	1752	VAL	N-CA-C	-6.20	104.30	110.62
2	A	1434	TYR	N-CA-C	-6.17	104.56	111.28
2	A	1318	ILE	N-CA-CB	6.03	114.30	110.50
2	A	1303	ARG	N-CA-C	6.02	117.84	111.28
1	C	127	CYS	CA-CB-SG	5.98	128.16	114.40
2	A	1249	GLY	N-CA-C	-5.98	105.14	112.68
2	A	293	LEU	N-CA-C	5.91	118.59	109.07
2	A	392	TYR	N-CA-C	5.85	117.46	111.14
1	C	132	PRO	O-C-N	5.84	123.90	121.15
2	A	148	PRO	O-C-N	5.81	123.98	121.31
2	A	1725	SER	N-CA-C	5.75	117.62	111.36
2	A	290	MET	N-CA-C	5.68	117.15	111.07
2	A	228	ILE	CA-C-N	-5.68	113.94	119.90
2	A	228	ILE	C-N-CA	-5.68	113.94	119.90
2	A	1499	ARG	CA-C-N	-5.68	113.85	119.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1499	ARG	C-N-CA	-5.68	113.85	119.92
2	A	145	MET	N-CA-C	5.67	117.46	111.28
2	A	148	PRO	CA-C-N	-5.67	114.42	120.03
2	A	148	PRO	C-N-CA	-5.67	114.42	120.03
2	A	1418	SER	N-CA-C	5.67	118.45	110.23
2	A	267	PHE	N-CA-C	5.61	120.12	112.88
2	A	1447	PHE	N-CA-C	5.61	117.19	111.14
2	A	745	PHE	N-CA-C	5.52	119.79	112.72
2	A	741	VAL	N-CA-C	-5.52	104.99	110.62
2	A	939	ALA	N-CA-C	5.47	119.95	113.28
2	A	887	LEU	N-CA-C	5.45	117.03	111.14
2	A	1342	LEU	N-CA-C	5.44	117.02	111.14
2	A	951	VAL	CB-CA-C	-5.43	104.81	112.14
2	A	317	PHE	N-CA-C	5.42	117.27	111.36
2	A	1318	ILE	CB-CA-C	-5.42	108.61	114.35
2	A	905	LEU	CA-C-N	-5.37	115.06	120.21
2	A	905	LEU	C-N-CA	-5.37	115.06	120.21
2	A	1363	GLN	N-CA-C	-5.33	101.43	109.85
2	A	306	LEU	N-CA-C	5.24	117.71	109.39
2	A	270	ASN	N-CA-C	5.22	117.05	111.36
2	A	752	ILE	N-CA-C	-5.20	105.32	110.62
2	A	1568	SER	N-CA-C	5.19	116.75	111.14
2	A	895	CYS	N-CA-C	5.19	117.01	111.36
2	A	266	LEU	N-CA-C	5.16	116.99	111.36
2	A	366	LEU	N-CA-C	-5.14	105.67	111.28
2	A	902	ASP	N-CA-C	5.12	116.87	111.28
2	A	1712	PRO	CA-C-O	-5.12	116.69	120.73
2	A	1732	ASN	N-CA-C	-5.11	102.14	109.24
3	B	125	ARG	N-CA-C	5.08	117.35	108.76
2	A	1708	LEU	N-CA-C	5.07	116.81	111.28
2	A	1288	SER	N-CA-C	-5.07	105.76	111.28
1	C	62	GLN	N-CA-C	5.06	116.87	111.36
2	A	1721	HIS	CA-C-N	-5.03	114.58	119.76
2	A	1721	HIS	C-N-CA	-5.03	114.58	119.76
2	A	1352	ASN	N-CA-C	-5.02	101.58	109.25
2	A	1449	LEU	N-CA-C	-5.01	105.82	111.28

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	943	141	0
2	A	9192	0	9424	1081	0
3	B	1416	0	1379	175	0
4	D	28	0	25	0	0
4	E	28	0	25	6	0
5	A	28	0	26	2	0
5	B	56	0	52	0	0
5	C	14	0	13	5	0
6	A	21	0	0	2	0
All	All	11763	0	11887	1385	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 59.

All (1385) 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	1.50
2:A:849:TRP:CD1	2:A:850:PRO:HD2	1.46	1.49
2:A:1694:ILE:CD1	2:A:1703:LEU:HD12	1.47	1.40
2:A:737:ILE:CG2	2:A:797:ALA:HB2	1.52	1.38
2:A:174:ARG:HD3	2:A:182:THR:CG2	1.55	1.37
1:C:65:LEU:CD1	1:C:110:VAL:HB	1.58	1.34
2:A:834:LEU:HD23	2:A:835:ARG:N	1.38	1.34
2:A:1694:ILE:HD11	2:A:1703:LEU:CD1	1.58	1.34
2:A:157:TYR:O	2:A:160:THR:HG22	1.20	1.33
2:A:1238:ILE:CD1	2:A:1270:LEU:HD23	1.59	1.32
2:A:849:TRP:HD1	2:A:850:PRO:CD	1.42	1.32
1:C:30:MET:HG3	1:C:138:GLY:CA	1.57	1.32
2:A:1497:ILE:CG2	2:A:1572:TYR:CD2	2.09	1.31
3:B:32:TYR:CD2	3:B:113:TYR:CE1	2.23	1.26
2:A:1496:PRO:O	2:A:1497:ILE:HD12	1.29	1.24
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:171:ILE:HG22	2:A:183:PHE:CE2	1.72	1.23

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:737:ILE:HB	2:A:797:ALA:CA	1.68	1.22
2:A:1238:ILE:HD11	2:A:1270:LEU:CD2	1.69	1.22
1:C:128:TYR:CD2	1:C:137:ARG:NH2	2.09	1.21
2:A:132:ILE:HD11	2:A:166:GLU:CB	1.68	1.20
2:A:839:LEU:O	2:A:842:VAL:HG23	1.41	1.20
2:A:293:LEU:HD12	2:A:298:ASP:CB	1.71	1.19
3:B:51:ALA:HB2	3:B:127:LEU:CD1	1.72	1.19
2:A:336:ASN:ND2	2:A:343:SER:HB3	1.56	1.19
2:A:737:ILE:CB	2:A:797:ALA:HB2	1.73	1.18
2:A:1732:ASN:HB3	2:A:1735:VAL:CG1	1.74	1.17
1:C:128:TYR:CD2	1:C:137:ARG:CZ	2.27	1.17
2:A:136:ILE:HD12	2:A:224:THR:HG22	1.22	1.17
2:A:293:LEU:CD1	2:A:298:ASP:HB3	1.72	1.17
2:A:174:ARG:HD3	2:A:182:THR:HG21	1.25	1.16
2:A:174:ARG:HB3	2:A:182:THR:HB	1.30	1.13
2:A:1212:GLU:O	2:A:1663:MET:HE1	1.48	1.13
2:A:737:ILE:HB	2:A:797:ALA:HA	1.22	1.12
2:A:1522:MET:HE1	2:A:1623:LEU:HD23	1.27	1.12
2:A:734:LYS:HE3	2:A:799:ASP:OD1	1.46	1.11
2:A:171:ILE:HG22	2:A:183:PHE:CD2	1.85	1.11
2:A:1502:ASN:HB3	2:A:1504:ILE:HD11	1.27	1.10
2:A:250:ILE:HG22	2:A:1630:ILE:HD11	1.28	1.10
2:A:149:PRO:O	2:A:152:THR:HG22	1.49	1.10
2:A:1639:MET:HA	2:A:1639:MET:HE2	1.20	1.10
2:A:960:LEU:CD2	2:A:964:LEU:HD23	1.82	1.10
2:A:737:ILE:HB	2:A:797:ALA:CB	1.82	1.09
1:C:30:MET:SD	1:C:137:ARG:CA	2.41	1.09
2:A:1522:MET:HE1	2:A:1623:LEU:CD2	1.81	1.09
2:A:798:MET:HE3	2:A:803:TYR:HA	1.34	1.09
2:A:794:LYS:HG2	2:A:803:TYR:CE1	1.87	1.08
2:A:1500:PRO:HG3	2:A:1505:GLN:HG2	1.13	1.08
2:A:794:LYS:HG2	2:A:803:TYR:HE1	0.97	1.08
3:B:32:TYR:CD2	3:B:113:TYR:HE1	1.64	1.08
2:A:810:ILE:O	2:A:814:LEU:HD12	1.53	1.08
3:B:60:ARG:HB3	3:B:66:GLU:O	1.53	1.08
2:A:795:LEU:HD11	2:A:803:TYR:CD2	1.89	1.08
2:A:174:ARG:CD	2:A:182:THR:HG22	1.83	1.07
2:A:822:GLU:OE2	2:A:835:ARG:HB2	1.54	1.07
2:A:960:LEU:HD23	2:A:964:LEU:HD23	1.34	1.06
2:A:1732:ASN:CB	2:A:1735:VAL:HG12	1.84	1.06
1:C:30:MET:SD	1:C:138:GLY:N	2.27	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1283:LEU:HD23	2:A:1283:LEU:H	1.19	1.06
2:A:136:ILE:CD1	2:A:224:THR:HG22	1.84	1.06
3:B:51:ALA:CB	3:B:127:LEU:CD1	2.32	1.06
2:A:132:ILE:HD11	2:A:166:GLU:HB3	1.31	1.05
1:C:30:MET:HG3	1:C:138:GLY:N	1.70	1.05
2:A:174:ARG:CD	2:A:182:THR:CG2	2.33	1.05
2:A:132:ILE:HD12	2:A:166:GLU:OE2	1.55	1.05
2:A:1764:SER:O	2:A:1767:THR:HG22	1.56	1.05
2:A:1541:GLN:OE1	2:A:1541:GLN:N	1.89	1.04
2:A:1498:PRO:CD	2:A:1572:TYR:CE2	2.40	1.04
2:A:1467:LEU:HD11	2:A:1472:ILE:HG23	1.40	1.04
2:A:1498:PRO:HD2	2:A:1572:TYR:HE2	1.21	1.04
3:B:54:PHE:CZ	3:B:124:TYR:HD2	1.76	1.04
1:C:65:LEU:HD11	1:C:110:VAL:HB	1.38	1.04
2:A:737:ILE:CG2	2:A:797:ALA:CB	2.35	1.04
1:C:101:PHE:CE2	1:C:103:GLY:O	2.11	1.03
2:A:737:ILE:HG22	2:A:797:ALA:HB2	1.05	1.03
2:A:1596:ALA:HB1	2:A:1609:PHE:CE2	1.93	1.03
2:A:1251:LYS:O	2:A:1255:THR:HG23	1.58	1.03
1:C:107:LYS:NZ	1:C:109:ASP:CB	2.20	1.03
2:A:795:LEU:CD1	2:A:803:TYR:CD2	2.41	1.03
2:A:737:ILE:HG22	2:A:797:ALA:CB	1.87	1.03
1:C:30:MET:SD	1:C:136:HIS:O	2.17	1.02
2:A:1485:MET:HB3	2:A:1639:MET:HE1	1.40	1.02
1:C:63:PHE:HE2	1:C:105:PRO:HB3	1.21	1.02
2:A:214:ARG:O	2:A:217:ARG:CG	2.07	1.02
2:A:399:ALA:CB	2:A:1762:ASN:HD22	1.73	1.01
2:A:737:ILE:CB	2:A:797:ALA:CB	2.37	1.01
2:A:214:ARG:O	2:A:217:ARG:HG3	1.61	1.00
3:B:60:ARG:CB	3:B:66:GLU:O	2.09	1.00
3:B:39:LEU:HD23	3:B:105:SER:OG	1.60	1.00
2:A:1485:MET:CB	2:A:1639:MET:HE1	1.92	1.00
2:A:1474:MET:HE2	2:A:1642:PRO:HB2	1.44	1.00
1:C:30:MET:SD	1:C:137:ARG:C	2.45	1.00
2:A:1498:PRO:HD3	2:A:1572:TYR:CE2	1.97	1.00
3:B:54:PHE:CZ	3:B:124:TYR:CD2	2.50	0.99
2:A:336:ASN:ND2	2:A:343:SER:CB	2.26	0.99
1:C:65:LEU:CD1	1:C:110:VAL:CB	2.39	0.99
2:A:1502:ASN:HB3	2:A:1504:ILE:CD1	1.91	0.99
3:B:32:TYR:HD2	3:B:113:TYR:CE1	1.69	0.99
2:A:822:GLU:CD	2:A:835:ARG:NH2	2.21	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1496:PRO:O	2:A:1497:ILE:CD1	2.12	0.98
1:C:30:MET:CG	1:C:138:GLY:N	2.27	0.98
1:C:62:GLN:O	1:C:132:PRO:CD	2.11	0.98
3:B:34:MET:O	3:B:111:VAL:HG23	1.64	0.98
1:C:31:GLU:HB3	1:C:53:ASN:HB3	1.45	0.98
2:A:1497:ILE:CG2	2:A:1572:TYR:HD2	1.65	0.98
2:A:1412:MET:HE2	2:A:1434:TYR:HE1	1.27	0.97
2:A:1374:MET:HG2	2:A:1380:VAL:HG13	1.46	0.97
2:A:1498:PRO:HD2	2:A:1572:TYR:CE2	2.00	0.97
2:A:133:MET:O	2:A:136:ILE:HG22	1.65	0.96
2:A:1498:PRO:CD	2:A:1572:TYR:HE2	1.77	0.96
2:A:157:TYR:O	2:A:160:THR:CG2	2.14	0.96
2:A:1212:GLU:O	2:A:1663:MET:CE	2.14	0.96
1:C:52:PHE:O	1:C:108:TYR:HB3	1.63	0.96
1:C:30:MET:SD	1:C:136:HIS:C	2.49	0.96
2:A:798:MET:CE	2:A:803:TYR:HA	1.94	0.96
1:C:128:TYR:HD2	1:C:137:ARG:CZ	1.74	0.95
2:A:1694:ILE:CD1	2:A:1703:LEU:CD1	2.27	0.95
3:B:57:TRP:CZ3	3:B:142:ILE:HD12	2.00	0.95
2:A:399:ALA:HB1	2:A:1762:ASN:ND2	1.81	0.95
2:A:399:ALA:CB	2:A:1762:ASN:ND2	2.30	0.95
2:A:1509:PHE:HB2	2:A:1568:SER:HB3	1.48	0.95
1:C:61:LYS:HG3	1:C:85:MET:HE1	1.49	0.95
3:B:32:TYR:CD2	3:B:113:TYR:CD1	2.56	0.94
2:A:1732:ASN:HB3	2:A:1735:VAL:HG12	0.95	0.94
1:C:30:MET:SD	1:C:137:ARG:HA	2.05	0.94
2:A:207:LEU:HD22	2:A:208:GLY:H	1.32	0.94
1:C:107:LYS:HZ3	1:C:109:ASP:CB	1.80	0.93
2:A:171:ILE:CG2	2:A:183:PHE:CE2	2.51	0.93
2:A:1238:ILE:CD1	2:A:1270:LEU:CD2	2.36	0.93
2:A:136:ILE:HD12	2:A:224:THR:CG2	1.97	0.93
1:C:79:MET:CE	5:C:301:NAG:C1	2.45	0.93
2:A:148:PRO:HB2	2:A:152:THR:HG21	1.49	0.93
2:A:164:THR:HG21	2:A:200:TYR:OH	1.67	0.92
1:C:52:PHE:HB2	1:C:129:ILE:HD13	1.51	0.92
1:C:79:MET:HE1	5:C:301:NAG:C1	2.00	0.92
2:A:822:GLU:CD	2:A:835:ARG:HH21	1.77	0.92
2:A:132:ILE:HD11	2:A:166:GLU:HB2	1.51	0.92
2:A:1430:SER:O	2:A:1432:TYR:N	2.04	0.91
1:C:66:ASN:ND2	1:C:79:MET:HE2	1.85	0.91
2:A:1500:PRO:CG	2:A:1505:GLN:HG2	1.99	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:838:ARG:HH11	2:A:838:ARG:HG3	1.35	0.91
2:A:967:LEU:CD2	2:A:968:LEU:HD13	2.01	0.91
3:B:57:TRP:CH2	3:B:142:ILE:CD1	2.54	0.91
2:A:207:LEU:HD22	2:A:208:GLY:N	1.85	0.91
2:A:1412:MET:HE2	2:A:1434:TYR:CE1	2.05	0.91
1:C:29:SER:N	1:C:136:HIS:CD2	2.39	0.90
2:A:136:ILE:CD1	2:A:224:THR:CG2	2.49	0.90
2:A:737:ILE:CB	2:A:797:ALA:CA	2.50	0.90
1:C:30:MET:HG3	1:C:138:GLY:HA2	1.53	0.90
1:C:135:ARG:HG2	1:C:135:ARG:HH21	1.36	0.90
1:C:62:GLN:O	1:C:132:PRO:HD3	1.71	0.90
2:A:132:ILE:HD12	2:A:166:GLU:CD	1.96	0.90
2:A:813:SER:O	2:A:817:THR:HG23	1.72	0.90
2:A:834:LEU:HD23	2:A:835:ARG:H	1.00	0.90
2:A:1504:ILE:HD13	2:A:1504:ILE:H	1.32	0.90
2:A:117:ARG:HB3	2:A:117:ARG:HH11	1.35	0.89
2:A:1497:ILE:HG23	2:A:1572:TYR:CE2	2.06	0.89
3:B:60:ARG:NH2	3:B:118:ASP:OD2	2.05	0.89
2:A:360:GLN:NE2	2:A:390:SER:OG	2.05	0.89
2:A:794:LYS:CG	2:A:803:TYR:HE1	1.85	0.89
2:A:250:ILE:CG2	2:A:1630:ILE:HD11	2.03	0.88
2:A:834:LEU:CD2	2:A:835:ARG:N	2.33	0.88
1:C:59:ASN:CB	1:C:62:GLN:HB2	2.03	0.88
2:A:1284:GLY:O	2:A:1287:LYS:N	2.06	0.88
1:C:63:PHE:HE1	1:C:129:ILE:CG2	1.86	0.88
3:B:57:TRP:CZ3	3:B:142:ILE:CD1	2.55	0.88
1:C:34:VAL:HG12	1:C:50:CYS:SG	2.13	0.88
3:B:32:TYR:HD2	3:B:113:TYR:CD1	1.91	0.88
2:A:174:ARG:HD2	2:A:182:THR:HG22	1.56	0.88
2:A:378:TYR:OH	2:A:1610:ARG:NH1	2.06	0.88
2:A:321:SER:HB3	2:A:375:GLY:HA2	1.52	0.88
2:A:834:LEU:CD2	2:A:835:ARG:H	1.87	0.88
3:B:119:TYR:HB2	3:B:142:ILE:O	1.74	0.88
2:A:742:MET:HB2	2:A:746:VAL:HB	1.54	0.87
1:C:52:PHE:CB	1:C:129:ILE:HD13	2.03	0.87
2:A:1581:PHE:O	2:A:1585:VAL:HG13	1.73	0.87
2:A:1639:MET:HA	2:A:1639:MET:CE	2.04	0.87
2:A:179:GLY:C	2:A:180:GLU:HG2	2.00	0.87
2:A:1290:ARG:HG2	2:A:1290:ARG:HH11	1.38	0.87
3:B:72:ARG:HH22	3:B:74:GLU:CD	1.81	0.87
2:A:1596:ALA:HB1	2:A:1609:PHE:HE2	1.36	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:841:ARG:HG2	2:A:841:ARG:HH11	1.39	0.86
2:A:1218:ARG:O	2:A:1219:LYS:HG2	1.75	0.86
2:A:1452:PHE:O	2:A:1456:ILE:HD12	1.75	0.86
2:A:117:ARG:HH11	2:A:117:ARG:CB	1.87	0.86
2:A:895:CYS:O	2:A:897:CYS:N	2.09	0.86
1:C:69:TYR:HE2	1:C:94:ARG:NH1	1.74	0.85
2:A:862:SER:O	2:A:870:THR:HG21	1.76	0.85
2:A:168:LEU:HD23	2:A:169:VAL:N	1.92	0.85
2:A:1520:SER:O	2:A:1523:VAL:HG12	1.76	0.85
2:A:179:GLY:O	2:A:180:GLU:CG	2.22	0.85
2:A:207:LEU:HD12	2:A:213:LEU:HD23	1.59	0.85
2:A:1186:TYR:O	2:A:1190:GLU:HG2	1.75	0.85
1:C:107:LYS:HZ2	1:C:109:ASP:CB	1.87	0.85
1:C:107:LYS:HZ2	1:C:109:ASP:HB3	1.41	0.85
1:C:107:LYS:NZ	1:C:109:ASP:CG	2.34	0.85
2:A:1457:ILE:HD12	2:A:1458:ASP:N	1.92	0.85
1:C:63:PHE:HE1	1:C:129:ILE:HG22	1.39	0.85
2:A:1384:ASN:OD1	2:A:1388:ASN:ND2	2.09	0.85
2:A:1532:MET:SD	2:A:1620:ILE:HD11	2.17	0.85
1:C:29:SER:N	1:C:136:HIS:HD2	1.74	0.85
2:A:795:LEU:CD1	2:A:803:TYR:CG	2.59	0.85
2:A:1288:SER:O	2:A:1291:THR:HG22	1.75	0.84
1:C:65:LEU:HD12	1:C:110:VAL:CB	2.08	0.84
1:C:66:ASN:ND2	1:C:79:MET:CE	2.39	0.84
1:C:107:LYS:HZ3	1:C:109:ASP:CG	1.84	0.84
2:A:214:ARG:O	2:A:217:ARG:HG2	1.76	0.84
2:A:1582:ASP:O	2:A:1585:VAL:HG22	1.77	0.84
2:A:1229:ALA:O	2:A:1232:ILE:HG22	1.76	0.84
2:A:1457:ILE:HG22	2:A:1756:ILE:CD1	2.07	0.84
2:A:276:PHE:CZ	2:A:280:LEU:HD21	2.12	0.84
1:C:33:THR:O	1:C:50:CYS:HA	1.79	0.83
2:A:1529:MET:HG2	2:A:1533:MET:HE3	1.59	0.83
3:B:46:ARG:HD3	3:B:48:GLU:OE2	1.78	0.83
1:C:63:PHE:CE2	1:C:105:PRO:HB3	2.09	0.83
2:A:1613:ARG:O	2:A:1616:ARG:HG2	1.76	0.83
2:A:1295:LEU:HD12	2:A:1298:LEU:HD22	1.60	0.83
2:A:1717:PRO:O	2:A:1728:GLY:HA3	1.79	0.83
3:B:85:ARG:HG2	3:B:85:ARG:HH11	1.43	0.83
2:A:736:CYS:O	2:A:740:ILE:HG12	1.78	0.83
2:A:869:LEU:HD12	2:A:869:LEU:O	1.78	0.83
1:C:107:LYS:HZ3	1:C:109:ASP:HB2	1.43	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1412:MET:CE	2:A:1434:TYR:CE1	2.62	0.83
2:A:1497:ILE:HG23	2:A:1572:TYR:CG	2.14	0.83
2:A:119:SER:O	2:A:122:ILE:HG22	1.79	0.82
3:B:34:MET:O	3:B:111:VAL:CG2	2.26	0.82
2:A:188:TRP:CD1	2:A:232:LYS:CE	2.61	0.82
2:A:1574:PHE:HD1	2:A:1580:ILE:HD11	1.45	0.82
1:C:30:MET:HG3	1:C:138:GLY:HA3	1.56	0.82
2:A:834:LEU:O	2:A:837:PHE:HB2	1.79	0.82
1:C:65:LEU:HD12	1:C:110:VAL:HB	1.61	0.82
2:A:366:LEU:O	2:A:370:THR:HG23	1.79	0.82
2:A:145:MET:HE3	2:A:145:MET:HA	1.62	0.81
2:A:1457:ILE:HG22	2:A:1756:ILE:HD11	1.61	0.81
4:E:1:NAG:H3	4:E:1:NAG:H83	1.61	0.81
2:A:399:ALA:HB1	2:A:1762:ASN:HD22	1.41	0.81
2:A:300:ARG:HH22	2:A:308:GLY:H	1.28	0.81
3:B:54:PHE:CE1	3:B:124:TYR:HD2	1.97	0.81
2:A:300:ARG:HH11	2:A:300:ARG:HG2	1.45	0.81
2:A:336:ASN:CG	2:A:343:SER:OG	2.24	0.81
2:A:1607:THR:HG23	2:A:1610:ARG:HH11	1.46	0.81
2:A:734:LYS:NZ	2:A:799:ASP:OD2	2.13	0.81
2:A:737:ILE:HG21	2:A:797:ALA:N	1.95	0.81
2:A:1460:PHE:HZ	2:A:1753:ASN:HD21	1.27	0.81
2:A:410:GLN:O	2:A:413:ILE:HG22	1.80	0.81
4:E:2:NAG:O7	4:E:2:NAG:O3	1.98	0.81
3:B:51:ALA:HB2	3:B:127:LEU:HD12	0.84	0.80
1:C:107:LYS:NZ	1:C:109:ASP:HB2	1.95	0.80
1:C:79:MET:HE2	5:C:301:NAG:O5	1.80	0.80
2:A:132:ILE:CD1	2:A:166:GLU:CB	2.56	0.80
2:A:327:GLY:O	3:B:132:TYR:HE2	1.64	0.80
2:A:835:ARG:HH21	2:A:835:ARG:HG3	1.46	0.80
3:B:85:ARG:O	3:B:115:HIS:HE1	1.63	0.80
2:A:281:GLU:O	2:A:284:GLU:HG3	1.82	0.80
3:B:57:TRP:HZ3	3:B:142:ILE:HD12	1.44	0.80
3:B:67:PHE:CE2	3:B:120:GLU:HG3	2.16	0.80
2:A:807:GLY:O	2:A:810:ILE:HG13	1.81	0.80
2:A:1522:MET:CE	2:A:1623:LEU:CD2	2.59	0.80
1:C:128:TYR:CG	1:C:137:ARG:NH2	2.49	0.80
2:A:412:ASN:O	2:A:415:GLU:HG3	1.82	0.80
2:A:1485:MET:HB3	2:A:1639:MET:CE	2.12	0.80
3:B:39:LEU:CD2	3:B:105:SER:OG	2.29	0.80
1:C:47:ARG:O	1:C:49:PRO:HD3	1.81	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:293:LEU:HD12	2:A:298:ASP:HB3	0.86	0.79
2:A:163:TYR:HA	2:A:166:GLU:HG2	1.64	0.79
2:A:116:ARG:HH12	2:A:176:PHE:CB	1.95	0.79
2:A:196:ILE:HD12	2:A:197:VAL:N	1.97	0.79
2:A:1293:ARG:CB	2:A:1293:ARG:HH21	1.94	0.79
2:A:1270:LEU:HD13	2:A:1270:LEU:O	1.83	0.79
2:A:188:TRP:CD1	2:A:232:LYS:HE3	2.18	0.79
1:C:33:THR:O	1:C:51:THR:N	2.15	0.78
2:A:160:THR:O	2:A:164:THR:HG23	1.83	0.78
2:A:1467:LEU:HD11	2:A:1472:ILE:CG2	2.12	0.78
2:A:315:CYS:HB3	2:A:324:CYS:SG	2.24	0.78
2:A:199:ALA:O	2:A:202:THR:HG22	1.84	0.78
2:A:795:LEU:HD12	2:A:803:TYR:CG	2.18	0.78
1:C:33:THR:HB	1:C:51:THR:CB	2.14	0.78
2:A:879:ILE:O	2:A:883:VAL:HG23	1.84	0.78
2:A:1709:ASN:HB2	2:A:1714:ASP:HB3	1.66	0.78
1:C:59:ASN:HB2	1:C:62:GLN:HB2	1.66	0.77
2:A:895:CYS:CB	2:A:938:VAL:HG12	2.15	0.77
2:A:1595:LEU:O	2:A:1599:ILE:HG13	1.83	0.77
2:A:1509:PHE:CB	2:A:1568:SER:HB3	2.14	0.77
1:C:62:GLN:O	1:C:132:PRO:HD2	1.85	0.77
2:A:1485:MET:SD	2:A:1639:MET:HE1	2.25	0.77
2:A:1755:TYR:O	2:A:1759:ILE:HG12	1.84	0.77
2:A:1637:LEU:HD22	2:A:1637:LEU:O	1.84	0.77
1:C:69:TYR:CE2	1:C:94:ARG:NH1	2.52	0.77
2:A:410:GLN:HE21	2:A:410:GLN:C	1.92	0.77
2:A:1677:ASP:OD2	3:B:46:ARG:NH1	2.18	0.77
2:A:136:ILE:HD13	2:A:136:ILE:O	1.84	0.77
4:E:1:NAG:H3	4:E:1:NAG:C8	2.14	0.77
2:A:765:HIS:HB2	2:A:767:PRO:HD2	1.65	0.77
3:B:51:ALA:HB1	3:B:126:LEU:O	1.85	0.77
3:B:92:TRP:CE2	3:B:94:GLY:HA3	2.20	0.77
2:A:116:ARG:HH12	2:A:176:PHE:HB2	1.48	0.77
2:A:207:LEU:HD12	2:A:213:LEU:CD2	2.14	0.76
2:A:321:SER:HB3	2:A:375:GLY:CA	2.15	0.76
1:C:52:PHE:HB2	1:C:129:ILE:CD1	2.15	0.76
1:C:107:LYS:HD2	1:C:109:ASP:HB2	1.67	0.76
1:C:59:ASN:HB3	1:C:62:GLN:HB2	1.68	0.76
2:A:131:LEU:HD22	2:A:131:LEU:O	1.84	0.76
1:C:79:MET:HE2	5:C:301:NAG:C1	2.11	0.76
3:B:32:TYR:CE2	3:B:113:TYR:CD1	2.74	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:851:THR:HG22	2:A:1327:VAL:HG21	1.66	0.76
3:B:71:LEU:HD21	3:B:106:ILE:HD12	1.68	0.76
2:A:188:TRP:CD1	2:A:232:LYS:HE2	2.20	0.76
2:A:806:VAL:CG2	2:A:809:ASN:HB2	2.16	0.76
1:C:31:GLU:O	1:C:52:PHE:HA	1.85	0.75
2:A:395:ASN:ND2	2:A:1755:TYR:CE1	2.53	0.75
2:A:1374:MET:CG	2:A:1380:VAL:HG13	2.15	0.75
1:C:65:LEU:HD13	1:C:110:VAL:HB	1.67	0.75
3:B:76:GLU:OE2	3:B:76:GLU:HA	1.86	0.75
2:A:737:ILE:CB	2:A:797:ALA:HA	2.09	0.75
3:B:32:TYR:CE2	3:B:113:TYR:CE1	2.74	0.75
1:C:32:VAL:HA	1:C:51:THR:O	1.86	0.75
2:A:755:VAL:O	2:A:758:THR:HG22	1.87	0.75
2:A:1213:ASP:HB3	2:A:1663:MET:HE3	1.67	0.75
2:A:1499:ARG:HG2	2:A:1509:PHE:CE1	2.22	0.75
3:B:72:ARG:NH2	3:B:74:GLU:OE2	2.20	0.75
1:C:135:ARG:HG2	1:C:135:ARG:NH2	2.00	0.75
2:A:407:GLU:HG3	2:A:408:GLN:N	2.02	0.75
2:A:909:HIS:HD2	2:A:911:ASN:H	1.34	0.75
2:A:145:MET:HE3	2:A:145:MET:CA	2.17	0.75
2:A:217:ARG:HB3	2:A:217:ARG:NH1	2.00	0.75
2:A:1290:ARG:HG2	2:A:1290:ARG:NH1	1.99	0.75
3:B:126:LEU:HD13	3:B:128:PHE:CZ	2.22	0.75
1:C:63:PHE:CE1	1:C:129:ILE:CG2	2.70	0.74
1:C:103:GLY:O	1:C:105:PRO:HD3	1.87	0.74
2:A:960:LEU:HD21	2:A:964:LEU:HD23	1.68	0.74
3:B:58:THR:HG22	3:B:69:LYS:HA	1.67	0.74
2:A:395:ASN:ND2	2:A:1755:TYR:CZ	2.55	0.74
1:C:58:VAL:HG13	1:C:63:PHE:HB2	1.69	0.74
2:A:1295:LEU:HD12	2:A:1298:LEU:CD2	2.17	0.74
2:A:210:VAL:O	2:A:214:ARG:HG2	1.87	0.74
2:A:1503:LYS:CD	2:A:1503:LYS:H	2.00	0.74
2:A:1497:ILE:HG21	2:A:1572:TYR:HD2	1.53	0.74
1:C:30:MET:SD	1:C:137:ARG:N	2.61	0.74
2:A:791:MET:HE3	2:A:795:LEU:HD22	1.70	0.74
2:A:1467:LEU:HD21	2:A:1472:ILE:CG2	2.18	0.74
2:A:1588:ILE:HG22	2:A:1615:ALA:HB1	1.70	0.74
2:A:896:VAL:O	2:A:899:ILE:HG12	1.87	0.74
2:A:838:ARG:HG3	2:A:838:ARG:NH1	2.03	0.74
2:A:207:LEU:C	2:A:207:LEU:HD13	2.13	0.73
2:A:1504:ILE:HG12	2:A:1505:GLN:N	2.03	0.73

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	2.11	0.73
2:A:118:ILE:HD13	2:A:118:ILE:N	2.04	0.73
2:A:167:SER:O	2:A:171:ILE:HG23	1.88	0.73
2:A:174:ARG:CB	2:A:182:THR:HB	2.16	0.73
2:A:116:ARG:HH12	2:A:176:PHE:CA	2.00	0.73
2:A:831:LEU:O	2:A:834:LEU:HD22	1.88	0.73
2:A:737:ILE:C	2:A:797:ALA:CB	2.61	0.73
1:C:101:PHE:HE2	1:C:103:GLY:O	1.69	0.73
2:A:835:ARG:NH2	2:A:835:ARG:HG3	2.00	0.73
2:A:1283:LEU:H	2:A:1283:LEU:CD2	1.99	0.73
2:A:1504:ILE:HD13	2:A:1504:ILE:N	2.03	0.73
2:A:1430:SER:HB3	2:A:1433:MET:HG2	1.70	0.72
2:A:1531:THR:O	2:A:1534:VAL:CG2	2.37	0.72
3:B:152:ARG:HG2	3:B:157:ILE:HG13	1.71	0.72
1:C:65:LEU:HD12	1:C:110:VAL:CG1	2.19	0.72
1:C:71:GLU:HG3	1:C:94:ARG:HH12	1.53	0.72
2:A:395:ASN:OD1	2:A:1755:TYR:CD1	2.41	0.72
2:A:1598:LEU:O	2:A:1601:THR:HG23	1.88	0.72
2:A:735:LYS:HD2	2:A:735:LYS:O	1.89	0.72
2:A:415:GLU:OE2	2:A:416:ALA:N	2.22	0.72
2:A:967:LEU:C	2:A:967:LEU:HD23	2.14	0.72
2:A:1336:SER:O	2:A:1340:VAL:HG23	1.89	0.72
3:B:60:ARG:HB2	3:B:66:GLU:O	1.88	0.72
1:C:41:LEU:HD23	1:C:147:LEU:HB3	1.71	0.72
2:A:116:ARG:NH1	2:A:176:PHE:HB2	2.05	0.72
2:A:318:SER:HB2	2:A:320:ASP:OD1	1.89	0.72
2:A:1597:ASP:O	2:A:1601:THR:HG22	1.90	0.72
3:B:85:ARG:O	3:B:115:HIS:CE1	2.43	0.72
2:A:1304:PHE:HD2	2:A:1307:MET:CE	2.01	0.72
2:A:787:PHE:CD1	2:A:841:ARG:NH1	2.57	0.72
3:B:92:TRP:CZ2	3:B:94:GLY:HA3	2.24	0.72
1:C:33:THR:HB	1:C:51:THR:OG1	1.90	0.71
2:A:168:LEU:HD23	2:A:168:LEU:C	2.15	0.71
3:B:54:PHE:CE2	3:B:124:TYR:HB2	2.25	0.71
3:B:72:ARG:NH2	3:B:74:GLU:CD	2.48	0.71
1:C:65:LEU:C	1:C:65:LEU:HD23	2.15	0.71
3:B:104:LEU:N	3:B:104:LEU:HD22	2.05	0.71
2:A:737:ILE:C	2:A:797:ALA:HB1	2.16	0.71
2:A:748:LEU:C	2:A:748:LEU:HD13	2.16	0.71
2:A:1295:LEU:CD1	2:A:1298:LEU:HD22	2.21	0.71
2:A:1365:PRO:O	2:A:1424:GLN:HB3	1.91	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:734:LYS:HE3	2:A:799:ASP:CG	2.15	0.71
2:A:841:ARG:HG2	2:A:841:ARG:NH1	2.04	0.71
2:A:1511:LEU:C	2:A:1511:LEU:HD23	2.16	0.71
2:A:399:ALA:HB3	2:A:1762:ASN:ND2	2.05	0.71
2:A:823:LEU:HD23	2:A:823:LEU:C	2.15	0.71
2:A:1273:LEU:HD12	2:A:1273:LEU:O	1.91	0.71
2:A:117:ARG:HA	2:A:120:ILE:HG22	1.73	0.71
2:A:171:ILE:HD12	2:A:171:ILE:C	2.15	0.71
2:A:822:GLU:CG	2:A:835:ARG:HH22	2.04	0.71
2:A:960:LEU:CD2	2:A:964:LEU:CD2	2.66	0.71
2:A:1286:ILE:HD12	2:A:1286:ILE:C	2.16	0.71
2:A:1504:ILE:CD1	2:A:1504:ILE:H	2.04	0.71
2:A:145:MET:HA	2:A:145:MET:CE	2.19	0.70
2:A:388:LEU:O	2:A:392:TYR:HB3	1.91	0.70
2:A:131:LEU:HD13	2:A:131:LEU:C	2.15	0.70
2:A:795:LEU:HD11	2:A:803:TYR:CE2	2.26	0.70
2:A:1261:LEU:O	2:A:1265:ILE:HG13	1.91	0.70
2:A:1317:ALA:O	2:A:1321:ILE:HG12	1.91	0.70
2:A:181:PHE:O	2:A:185:ARG:HG2	1.91	0.70
2:A:388:LEU:HD13	2:A:388:LEU:C	2.16	0.70
1:C:107:LYS:NZ	1:C:109:ASP:OD2	2.24	0.70
2:A:196:ILE:HD12	2:A:196:ILE:C	2.16	0.70
2:A:902:ASP:O	2:A:903:CYS:HB2	1.90	0.70
2:A:1764:SER:C	2:A:1767:THR:HG22	2.16	0.70
2:A:823:LEU:HD23	2:A:823:LEU:O	1.90	0.70
2:A:726:CYS:HB2	2:A:728:PRO:HD2	1.71	0.70
2:A:790:GLU:HG3	2:A:791:MET:N	2.05	0.70
2:A:791:MET:HG2	2:A:803:TYR:OH	1.92	0.70
2:A:1574:PHE:HD1	2:A:1580:ILE:CD1	2.04	0.70
2:A:852:LEU:HD13	2:A:1327:VAL:HG13	1.72	0.70
3:B:125:ARG:NH1	3:B:125:ARG:HG3	2.06	0.70
2:A:793:LEU:C	2:A:793:LEU:HD13	2.16	0.70
2:A:1221:THR:O	2:A:1224:ILE:HG22	1.92	0.70
3:B:86:PHE:HZ	3:B:119:TYR:HH	1.40	0.70
2:A:166:GLU:HG3	2:A:167:SER:N	2.08	0.69
2:A:1375:ASN:OD1	5:A:2005:NAG:O5	2.03	0.69
2:A:1457:ILE:HD12	2:A:1457:ILE:C	2.16	0.69
3:B:187:ALA:O	3:B:190:GLU:HG3	1.92	0.69
2:A:123:LEU:HD23	2:A:123:LEU:O	1.92	0.69
2:A:136:ILE:HD13	2:A:136:ILE:C	2.17	0.69
1:C:71:GLU:CG	1:C:94:ARG:HH12	2.06	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1238:ILE:HD11	2:A:1270:LEU:HD23	0.75	0.69
3:B:152:ARG:HG2	3:B:157:ILE:CG1	2.22	0.69
2:A:336:ASN:HD21	2:A:343:SER:HB3	1.55	0.69
2:A:1200:LEU:HD23	2:A:1201:MET:HE2	1.74	0.69
3:B:71:LEU:CD2	3:B:106:ILE:HD12	2.21	0.69
1:C:33:THR:HB	1:C:51:THR:HB	1.73	0.69
2:A:761:MET:HE1	2:A:839:LEU:HB3	1.75	0.69
3:B:71:LEU:CD2	3:B:106:ILE:CD1	2.70	0.69
2:A:1650:LEU:HD13	2:A:1650:LEU:O	1.93	0.69
3:B:27:GLU:OE2	3:B:27:GLU:HA	1.92	0.69
1:C:33:THR:N	1:C:51:THR:O	2.26	0.68
2:A:795:LEU:CD1	2:A:803:TYR:CE2	2.76	0.68
2:A:207:LEU:HD21	2:A:209:ASN:OD1	1.93	0.68
2:A:822:GLU:OE2	2:A:835:ARG:CB	2.38	0.68
2:A:1528:ASN:HD22	2:A:1528:ASN:C	2.02	0.68
2:A:262:ILE:HG12	2:A:1617:ILE:HD12	1.75	0.68
2:A:840:LEU:O	2:A:842:VAL:N	2.25	0.68
2:A:1561:GLU:HG3	2:A:1562:CYS:N	2.07	0.68
3:B:125:ARG:HG3	3:B:125:ARG:HH11	1.59	0.68
2:A:207:LEU:HD11	2:A:209:ASN:OD1	1.93	0.68
2:A:834:LEU:HD23	2:A:834:LEU:C	2.14	0.68
2:A:1474:MET:CE	2:A:1642:PRO:HB2	2.19	0.68
2:A:293:LEU:HD11	2:A:298:ASP:C	2.18	0.68
2:A:1286:ILE:O	2:A:1289:LEU:HB2	1.93	0.68
2:A:1694:ILE:HD12	2:A:1703:LEU:CD1	2.22	0.68
2:A:1750:VAL:O	2:A:1753:ASN:HB2	1.93	0.68
3:B:112:THR:HG22	3:B:113:TYR:N	2.08	0.68
2:A:822:GLU:CG	2:A:835:ARG:NH2	2.57	0.68
2:A:1619:ARG:O	2:A:1622:ARG:HG3	1.94	0.68
2:A:207:LEU:CD1	2:A:213:LEU:HD23	2.23	0.67
2:A:1650:LEU:HD13	2:A:1650:LEU:C	2.18	0.67
1:C:30:MET:CG	1:C:138:GLY:CA	2.52	0.67
2:A:276:PHE:HZ	2:A:280:LEU:HD21	1.55	0.67
2:A:1304:PHE:CD2	2:A:1307:MET:CE	2.77	0.67
2:A:217:ARG:HB3	2:A:217:ARG:CZ	2.24	0.67
2:A:1412:MET:CE	2:A:1434:TYR:CD1	2.77	0.67
2:A:191:LEU:O	2:A:191:LEU:HD23	1.95	0.67
2:A:264:LEU:O	2:A:268:MET:HB3	1.95	0.67
3:B:50:ASN:O	3:B:50:ASN:ND2	2.28	0.67
1:C:34:VAL:HG23	1:C:142:ILE:HG12	1.76	0.67
2:A:812:ASP:OD2	2:A:844:LYS:NZ	2.22	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:773:LYS:HE3	2:A:773:LYS:O	1.94	0.67
3:B:73:TYR:CD1	3:B:78:LEU:HB2	2.29	0.67
2:A:332:LYS:HG3	2:A:332:LYS:O	1.95	0.67
2:A:817:THR:O	2:A:821:VAL:HG23	1.95	0.67
2:A:1287:LYS:HD3	2:A:1287:LYS:C	2.19	0.67
3:B:69:LYS:NZ	3:B:81:GLU:OE2	2.28	0.67
1:C:79:MET:CE	5:C:301:NAG:O5	2.43	0.66
2:A:822:GLU:HG2	2:A:835:ARG:HH22	1.59	0.66
2:A:960:LEU:HD23	2:A:960:LEU:O	1.95	0.66
2:A:895:CYS:HB2	2:A:938:VAL:HG12	1.76	0.66
3:B:57:TRP:CH2	3:B:142:ILE:HD11	2.29	0.66
3:B:98:THR:O	3:B:99:LYS:HB3	1.95	0.66
2:A:290:MET:HE2	2:A:333:ILE:HG22	1.77	0.66
2:A:881:ALA:O	2:A:916:SER:OG	2.13	0.66
2:A:116:ARG:HH12	2:A:176:PHE:HA	1.60	0.66
2:A:737:ILE:HG21	2:A:797:ALA:H	1.60	0.66
2:A:1218:ARG:HG2	2:A:1218:ARG:HH21	1.60	0.66
2:A:1363:GLN:O	2:A:1364:VAL:HG12	1.96	0.66
2:A:787:PHE:CE1	2:A:841:ARG:NH1	2.64	0.66
2:A:1412:MET:CE	2:A:1434:TYR:HE1	1.99	0.66
2:A:136:ILE:HD11	2:A:224:THR:CG2	2.25	0.66
2:A:251:LEU:HD13	2:A:1630:ILE:HG23	1.77	0.66
2:A:772:PHE:HE1	2:A:776:LEU:HD23	1.60	0.66
2:A:1202:ILE:O	2:A:1206:SER:OG	2.14	0.66
2:A:772:PHE:CE1	2:A:776:LEU:HD23	2.31	0.66
1:C:65:LEU:CD1	1:C:110:VAL:CG1	2.74	0.66
2:A:192:ASP:OD1	2:A:223:LYS:HD2	1.96	0.66
2:A:1318:ILE:CG1	2:A:1319:PRO:HD3	2.26	0.66
2:A:1318:ILE:HG13	2:A:1319:PRO:HD3	1.76	0.65
2:A:1500:PRO:HG3	2:A:1505:GLN:CG	2.08	0.65
2:A:367:TYR:OH	2:A:1689:ILE:HG23	1.96	0.65
1:C:62:GLN:C	1:C:132:PRO:HD2	2.21	0.65
1:C:65:LEU:HD12	1:C:110:VAL:HG11	1.77	0.65
2:A:928:TRP:CZ3	2:A:929:ILE:HD12	2.31	0.65
2:A:220:ARG:O	2:A:223:LYS:HB2	1.97	0.65
2:A:336:ASN:CB	2:A:343:SER:OG	2.45	0.65
2:A:895:CYS:HB3	2:A:938:VAL:HG12	1.78	0.65
2:A:196:ILE:O	2:A:200:TYR:HD1	1.79	0.65
2:A:202:THR:OG1	2:A:214:ARG:NH1	2.30	0.64
2:A:361:ASP:OD2	2:A:929:ILE:HG22	1.97	0.64
2:A:843:PHE:O	2:A:845:LEU:N	2.31	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1214:ILE:HD12	3:B:22:VAL:CG2	2.27	0.64
2:A:1602:TYR:O	2:A:1603:PHE:HB2	1.96	0.64
2:A:131:LEU:HD13	2:A:132:ILE:N	2.12	0.64
2:A:132:ILE:CD1	2:A:166:GLU:HB2	2.26	0.64
2:A:332:LYS:O	2:A:333:ILE:HG12	1.97	0.64
2:A:764:GLU:OE1	2:A:1341:ASN:ND2	2.31	0.64
2:A:798:MET:HE2	2:A:803:TYR:CD1	2.33	0.64
2:A:851:THR:CG2	2:A:1327:VAL:HG21	2.27	0.64
3:B:73:TYR:HD1	3:B:78:LEU:HB2	1.62	0.64
2:A:1635:PHE:CE1	2:A:1638:MET:HE1	2.32	0.64
2:A:157:TYR:C	2:A:160:THR:HG22	2.15	0.64
2:A:209:ASN:OD1	2:A:209:ASN:N	2.30	0.64
2:A:909:HIS:CD2	2:A:911:ASN:H	2.15	0.64
2:A:947:VAL:O	2:A:951:VAL:HG23	1.98	0.64
2:A:1460:PHE:CZ	2:A:1753:ASN:ND2	2.66	0.64
2:A:250:ILE:HG22	2:A:1630:ILE:CD1	2.18	0.64
2:A:300:ARG:NH2	2:A:308:GLY:H	1.96	0.64
2:A:945:LEU:O	2:A:949:MET:HG2	1.98	0.64
2:A:119:SER:OG	2:A:173:ALA:HB2	1.97	0.64
2:A:1431:LEU:HD12	2:A:1431:LEU:O	1.98	0.64
2:A:1450:ASN:HD22	2:A:1450:ASN:C	2.06	0.64
2:A:1732:ASN:CB	2:A:1735:VAL:CG1	2.61	0.64
2:A:866:LEU:O	2:A:870:THR:HG22	1.97	0.64
1:C:61:LYS:HG3	1:C:85:MET:CE	2.24	0.64
2:A:1293:ARG:HH21	2:A:1293:ARG:HB2	1.63	0.64
2:A:1385:LEU:O	2:A:1386:LYS:HB2	1.96	0.64
2:A:1467:LEU:HD21	2:A:1472:ILE:HG21	1.79	0.64
2:A:1760:LEU:HD23	2:A:1760:LEU:O	1.98	0.64
2:A:867:GLY:HA2	2:A:870:THR:CG2	2.28	0.63
2:A:1251:LYS:O	2:A:1255:THR:CG2	2.40	0.63
2:A:1304:PHE:CD2	2:A:1307:MET:HE1	2.33	0.63
2:A:1491:LYS:O	2:A:1491:LYS:HD3	1.98	0.63
2:A:936:MET:CE	2:A:945:LEU:CD1	2.77	0.63
2:A:1742:SER:O	2:A:1746:ILE:HG13	1.98	0.63
3:B:46:ARG:NH2	3:B:48:GLU:OE2	2.27	0.63
2:A:117:ARG:CA	2:A:120:ILE:HG22	2.28	0.63
2:A:132:ILE:HG22	2:A:227:VAL:HG11	1.81	0.63
2:A:793:LEU:HD13	2:A:793:LEU:O	1.98	0.63
2:A:960:LEU:HD21	2:A:964:LEU:CD2	2.29	0.63
2:A:1364:VAL:HG23	2:A:1370:CYS:HA	1.80	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:1609:PHE:CE1	2:A:1613:ARG:HD2	2.33	0.63
2:A:1671:LYS:NZ	2:A:1682:GLU:OE2	2.32	0.63
2:A:1218:ARG:O	2:A:1219:LYS:CG	2.46	0.63
2:A:1485:MET:SD	2:A:1639:MET:CE	2.87	0.63
3:B:86:PHE:HZ	3:B:119:TYR:OH	1.80	0.63
1:C:103:GLY:HA3	1:C:109:ASP:OD1	1.99	0.62
2:A:754:ILE:HG12	2:A:787:PHE:CE1	2.33	0.62
2:A:798:MET:O	2:A:802:GLU:HB2	1.99	0.62
2:A:1522:MET:CE	2:A:1623:LEU:HD23	2.16	0.62
2:A:849:TRP:HD1	2:A:850:PRO:HD2	0.56	0.62
2:A:1514:ASN:HD22	2:A:1515:GLN:N	1.97	0.62
2:A:960:LEU:HD23	2:A:964:LEU:CD2	2.22	0.62
2:A:962:LEU:O	2:A:966:LEU:HB2	2.00	0.62
2:A:1294:ALA:O	2:A:1297:PRO:HD2	2.00	0.62
2:A:822:GLU:HG2	2:A:835:ARG:NH2	2.14	0.62
2:A:1353:THR:HB	2:A:1379:ASN:O	2.00	0.62
2:A:1497:ILE:CG2	2:A:1572:TYR:CE2	2.76	0.62
2:A:737:ILE:C	2:A:797:ALA:HB2	2.25	0.62
2:A:266:LEU:O	2:A:1610:ARG:NH2	2.33	0.62
2:A:321:SER:HB2	2:A:372:ARG:O	1.99	0.62
2:A:1504:ILE:HG12	2:A:1505:GLN:H	1.65	0.62
1:C:34:VAL:CG2	1:C:142:ILE:HG12	2.29	0.62
2:A:1582:ASP:OD1	2:A:1622:ARG:CZ	2.47	0.62
3:B:28:THR:HG22	3:B:143:HIS:O	2.00	0.62
3:B:40:CYS:O	3:B:104:LEU:O	2.16	0.62
2:A:148:PRO:CB	2:A:152:THR:HG21	2.28	0.62
2:A:1219:LYS:HG3	2:A:1219:LYS:O	2.00	0.61
3:B:53:THR:HG22	3:B:54:PHE:N	2.15	0.61
2:A:139:ASN:C	2:A:139:ASN:HD22	2.06	0.61
2:A:117:ARG:HH11	2:A:117:ARG:CG	2.12	0.61
2:A:1308:ARG:CB	2:A:1308:ARG:HH21	2.13	0.61
2:A:1531:THR:O	2:A:1534:VAL:HG23	1.99	0.61
2:A:812:ASP:O	2:A:816:VAL:HG23	2.00	0.61
2:A:862:SER:O	2:A:870:THR:CG2	2.48	0.61
3:B:153:ASP:OD1	3:B:154:MET:N	2.34	0.61
2:A:178:VAL:HG12	2:A:178:VAL:O	1.99	0.61
2:A:221:ALA:O	2:A:224:THR:HG23	2.01	0.61
2:A:1318:ILE:HG13	2:A:1319:PRO:CD	2.29	0.61
2:A:1599:ILE:O	2:A:1603:PHE:N	2.30	0.61
3:B:51:ALA:CB	3:B:127:LEU:HD13	2.30	0.61
2:A:1367:ARG:HB2	2:A:1382:TRP:CZ2	2.36	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:LEU:HD21	1:C:67:TRP:CD1	2.35	0.61
2:A:737:ILE:CG2	2:A:797:ALA:N	2.63	0.61
2:A:967:LEU:HD23	2:A:968:LEU:N	2.16	0.61
1:C:59:ASN:O	1:C:63:PHE:N	2.30	0.61
1:C:105:PRO:HA	1:C:109:ASP:O	2.01	0.61
2:A:783:PHE:O	2:A:787:PHE:HD2	1.83	0.61
2:A:349:TRP:HA	2:A:349:TRP:CE3	2.36	0.60
2:A:849:TRP:CD1	2:A:850:PRO:CD	2.35	0.60
2:A:840:LEU:C	2:A:842:VAL:N	2.57	0.60
2:A:1555:ILE:HD12	2:A:1593:MET:CE	2.31	0.60
2:A:1707:ILE:HG21	2:A:1736:GLY:HA3	1.84	0.60
2:A:132:ILE:CD1	2:A:166:GLU:OE2	2.43	0.60
2:A:738:TYR:N	2:A:797:ALA:HB1	2.17	0.60
2:A:1217:GLU:OE1	2:A:1217:GLU:HA	2.00	0.60
3:B:51:ALA:HB2	3:B:127:LEU:HA	1.83	0.60
2:A:835:ARG:HH21	2:A:835:ARG:CG	2.14	0.60
2:A:945:LEU:HD23	2:A:949:MET:HE3	1.84	0.60
2:A:839:LEU:HD13	2:A:1334:ILE:HG23	1.84	0.60
2:A:1457:ILE:HG22	2:A:1756:ILE:HD12	1.81	0.60
3:B:38:ILE:HG22	3:B:142:ILE:HD13	1.82	0.60
3:B:82:GLU:OE1	3:B:82:GLU:N	2.35	0.60
2:A:1218:ARG:HG2	3:B:23:GLU:O	2.02	0.60
2:A:1498:PRO:HD3	2:A:1572:TYR:CZ	2.37	0.60
3:B:55:THR:HG22	3:B:56:GLU:N	2.16	0.60
2:A:967:LEU:HD22	2:A:968:LEU:HD13	1.83	0.60
2:A:1179:TRP:CD1	2:A:1183:LYS:HE2	2.37	0.60
2:A:168:LEU:O	2:A:171:ILE:HG13	2.02	0.59
2:A:262:ILE:HG12	2:A:1617:ILE:CD1	2.32	0.59
2:A:337:PRO:O	2:A:338:ASP:HB2	2.02	0.59
2:A:1364:VAL:O	2:A:1364:VAL:HG13	2.00	0.59
3:B:57:TRP:HH2	3:B:142:ILE:CD1	2.09	0.59
3:B:165:VAL:O	3:B:169:VAL:HG23	2.02	0.59
2:A:132:ILE:CD1	2:A:166:GLU:CD	2.71	0.59
2:A:822:GLU:OE1	2:A:835:ARG:NH2	2.35	0.59
2:A:1218:ARG:HH21	2:A:1218:ARG:CG	2.14	0.59
2:A:971:PHE:CE2	2:A:1458:ASP:OD2	2.56	0.59
2:A:1280:TYR:CE1	2:A:1283:LEU:HD11	2.37	0.59
2:A:1308:ARG:HH21	2:A:1308:ARG:HB2	1.67	0.59
2:A:1608:LEU:O	2:A:1612:ILE:HG12	2.03	0.59
2:A:1635:PHE:CE1	2:A:1638:MET:CE	2.86	0.59
3:B:129:PHE:HB2	3:B:132:TYR:HB3	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:174:ARG:HD3	2:A:182:THR:CB	2.29	0.59
2:A:1508:ILE:O	2:A:1512:VAL:HG23	2.03	0.59
2:A:1572:TYR:O	2:A:1575:THR:HG23	2.03	0.59
2:A:300:ARG:HG2	2:A:300:ARG:NH1	2.17	0.59
2:A:1509:PHE:HA	2:A:1568:SER:CB	2.32	0.59
3:B:125:ARG:HH11	3:B:125:ARG:CG	2.15	0.59
2:A:171:ILE:CG2	2:A:183:PHE:CD2	2.75	0.59
2:A:765:HIS:CD2	2:A:768:MET:HG3	2.38	0.59
3:B:32:TYR:CE2	3:B:113:TYR:HD1	2.17	0.59
2:A:1497:ILE:HG21	2:A:1572:TYR:CD2	2.24	0.59
2:A:1270:LEU:HD13	2:A:1270:LEU:C	2.26	0.58
2:A:1504:ILE:O	2:A:1508:ILE:HG13	2.03	0.58
2:A:207:LEU:CD1	2:A:209:ASN:H	2.16	0.58
2:A:389:GLY:O	2:A:393:LEU:HB2	2.03	0.58
2:A:1503:LYS:H	2:A:1503:LYS:HD2	1.66	0.58
1:C:31:GLU:O	1:C:53:ASN:N	2.37	0.58
2:A:295:SER:HB3	2:A:298:ASP:HB2	1.86	0.58
2:A:748:LEU:HD13	2:A:749:ALA:N	2.18	0.58
2:A:1318:ILE:N	2:A:1319:PRO:HD2	2.18	0.58
2:A:1408:TRP:CD1	2:A:1409:THR:HG23	2.39	0.58
2:A:1496:PRO:O	2:A:1497:ILE:CG1	2.51	0.58
1:C:65:LEU:HD23	1:C:65:LEU:O	2.04	0.58
1:C:65:LEU:HD21	1:C:67:TRP:HD1	1.67	0.58
2:A:748:LEU:HD22	2:A:748:LEU:O	2.04	0.58
2:A:1551:ASN:O	2:A:1555:ILE:HG13	2.03	0.58
2:A:742:MET:HB2	2:A:746:VAL:CB	2.30	0.58
2:A:1200:LEU:HD23	2:A:1201:MET:CE	2.34	0.58
2:A:145:MET:HE3	2:A:145:MET:N	2.18	0.58
2:A:287:GLU:HA	2:A:287:GLU:OE1	2.03	0.58
3:B:177:GLU:HA	3:B:177:GLU:OE1	2.04	0.58
2:A:247:ASP:OD1	2:A:1629:GLY:C	2.47	0.58
2:A:153:LYS:HE3	2:A:157:TYR:OH	2.04	0.58
2:A:772:PHE:HE1	2:A:776:LEU:CD2	2.16	0.58
2:A:806:VAL:HG23	2:A:809:ASN:HB2	1.86	0.58
2:A:831:LEU:N	2:A:831:LEU:HD22	2.19	0.58
2:A:936:MET:CE	2:A:945:LEU:HD12	2.34	0.58
2:A:967:LEU:HD23	2:A:968:LEU:HD13	1.82	0.58
2:A:1717:PRO:O	2:A:1728:GLY:CA	2.51	0.58
2:A:810:ILE:HG13	2:A:811:PHE:N	2.18	0.57
2:A:1318:ILE:CG1	2:A:1319:PRO:CD	2.82	0.57
2:A:336:ASN:HD22	2:A:343:SER:HB3	1.61	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:737:ILE:CG2	2:A:797:ALA:CA	2.78	0.57
2:A:815:ILE:HD13	2:A:815:ILE:N	2.19	0.57
2:A:1179:TRP:NE1	2:A:1183:LYS:HE2	2.19	0.57
2:A:1218:ARG:HB3	2:A:1218:ARG:NH2	2.18	0.57
2:A:1539:GLN:O	2:A:1540:SER:OG	2.16	0.57
2:A:1637:LEU:HD22	2:A:1637:LEU:C	2.28	0.57
3:B:78:LEU:HD21	3:B:80:LEU:HD13	1.85	0.57
2:A:123:LEU:HD23	2:A:123:LEU:C	2.29	0.57
2:A:839:LEU:O	2:A:842:VAL:CG2	2.34	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
2:A:197:VAL:O	2:A:201:LEU:N	2.32	0.57
2:A:1764:SER:O	2:A:1767:THR:CG2	2.41	0.57
2:A:383:VAL:O	2:A:387:PHE:HB2	2.04	0.57
2:A:1359:PHE:HB3	2:A:1360:PRO:HD2	1.85	0.57
2:A:1440:PHE:O	2:A:1444:GLY:N	2.34	0.57
3:B:67:PHE:HE2	3:B:120:GLU:HG3	1.69	0.57
3:B:84:GLU:HA	3:B:87:GLU:HB2	1.87	0.57
2:A:1263:PHE:O	2:A:1266:VAL:HG12	2.05	0.57
2:A:1598:LEU:HA	2:A:1601:THR:CG2	2.34	0.57
2:A:1668:TYR:O	2:A:1729:ASP:CB	2.52	0.57
2:A:1545:GLU:OE1	2:A:1545:GLU:HA	2.03	0.57
2:A:192:ASP:O	2:A:196:ILE:HG23	2.05	0.57
2:A:790:GLU:O	2:A:794:LYS:HB2	2.04	0.57
2:A:836:SER:O	2:A:839:LEU:HG	2.04	0.57
2:A:1185:CYS:O	2:A:1189:VAL:HG22	2.04	0.57
2:A:1531:THR:O	2:A:1534:VAL:HG22	2.04	0.57
2:A:278:ASN:HD21	2:A:329:THR:CB	2.18	0.57
3:B:51:ALA:CB	3:B:126:LEU:O	2.53	0.57
2:A:193:PHE:O	2:A:196:ILE:HG13	2.04	0.56
2:A:936:MET:HE2	2:A:945:LEU:HD12	1.85	0.56
3:B:85:ARG:HH11	3:B:85:ARG:CG	2.14	0.56
3:B:187:ALA:HA	3:B:190:GLU:OE1	2.04	0.56
2:A:414:GLU:HG3	2:A:415:GLU:N	2.19	0.56
2:A:738:TYR:O	2:A:741:VAL:HG13	2.06	0.56
2:A:789:ALA:O	2:A:792:VAL:HG12	2.05	0.56
2:A:1304:PHE:HD2	2:A:1307:MET:HE1	1.69	0.56
2:A:1694:ILE:HD11	2:A:1703:LEU:HD12	0.64	0.56
2:A:1703:LEU:O	2:A:1706:PRO:HD2	2.05	0.56
3:B:75:ASN:CG	3:B:76:GLU:H	2.13	0.56
2:A:163:TYR:O	2:A:167:SER:HB2	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:46:ARG:HB3	3:B:48:GLU:OE2	2.05	0.56
2:A:116:ARG:O	2:A:120:ILE:HG22	2.06	0.56
2:A:320:ASP:OD1	2:A:320:ASP:N	2.39	0.56
2:A:1212:GLU:O	2:A:1213:ASP:HB3	2.05	0.56
2:A:1350:CYS:HB2	2:A:1424:GLN:HE22	1.71	0.56
2:A:1704:LEU:HD22	2:A:1708:LEU:HG	1.88	0.56
2:A:843:PHE:O	2:A:846:ALA:N	2.27	0.56
2:A:1206:SER:O	2:A:1209:LEU:HB2	2.05	0.56
2:A:971:PHE:HE2	2:A:1458:ASP:OD2	1.88	0.56
2:A:737:ILE:CA	2:A:797:ALA:HB2	2.36	0.56
2:A:1325:LEU:CD1	2:A:1329:LEU:HG	2.35	0.56
2:A:184:LEU:HD11	2:A:190:TRP:CD1	2.41	0.56
1:C:101:PHE:CZ	1:C:103:GLY:O	2.56	0.56
2:A:327:GLY:O	3:B:132:TYR:CE2	2.52	0.56
2:A:1358:ARG:NH1	2:A:1417:ASP:OD2	2.37	0.56
1:C:107:LYS:O	1:C:108:TYR:HB2	2.06	0.55
2:A:336:ASN:ND2	2:A:343:SER:OG	2.38	0.55
2:A:840:LEU:O	2:A:841:ARG:C	2.48	0.55
2:A:1704:LEU:HD22	2:A:1704:LEU:O	2.06	0.55
2:A:1358:ARG:NH2	2:A:1417:ASP:OD2	2.38	0.55
2:A:1589:SER:OG	2:A:1619:ARG:NH2	2.40	0.55
3:B:32:TYR:CD1	3:B:32:TYR:C	2.85	0.55
1:C:44:SER:O	1:C:117:VAL:HG22	2.07	0.55
2:A:117:ARG:C	2:A:120:ILE:HG22	2.32	0.55
2:A:843:PHE:O	2:A:844:LYS:C	2.48	0.55
2:A:207:LEU:HD13	2:A:209:ASN:N	2.22	0.55
2:A:278:ASN:ND2	2:A:329:THR:HB	2.21	0.55
2:A:734:LYS:CE	2:A:799:ASP:CG	2.80	0.55
2:A:806:VAL:HG23	2:A:809:ASN:CB	2.37	0.55
2:A:1321:ILE:HD11	2:A:1456:ILE:HG12	1.89	0.55
3:B:74:GLU:O	3:B:75:ASN:HB3	2.05	0.55
3:B:91:VAL:HG23	3:B:107:PHE:HB3	1.88	0.55
2:A:293:LEU:HD12	2:A:298:ASP:CG	2.30	0.55
3:B:67:PHE:CD1	3:B:67:PHE:N	2.73	0.55
2:A:405:TYR:CD1	2:A:405:TYR:C	2.85	0.55
2:A:832:SER:O	2:A:835:ARG:HB3	2.06	0.55
2:A:1635:PHE:HE1	2:A:1638:MET:HE1	1.71	0.55
3:B:46:ARG:HH21	3:B:48:GLU:CD	2.14	0.55
2:A:849:TRP:CH2	2:A:1326:LEU:HB3	2.42	0.55
2:A:1283:LEU:HD23	2:A:1283:LEU:N	2.03	0.55
2:A:1514:ASN:ND2	2:A:1516:ALA:H	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:151:TRP:CE3	2:A:151:TRP:C	2.85	0.54
2:A:286:LEU:HD22	2:A:286:LEU:O	2.07	0.54
2:A:806:VAL:HG23	2:A:809:ASN:H	1.72	0.54
3:B:48:GLU:HG2	3:B:49:THR:N	2.22	0.54
2:A:116:ARG:NH1	2:A:176:PHE:CB	2.65	0.54
2:A:766:HIS:CD2	2:A:766:HIS:C	2.86	0.54
2:A:1512:VAL:HG11	2:A:1565:LYS:HG3	1.89	0.54
2:A:1640:SER:HB3	2:A:1761:GLU:HG3	1.89	0.54
2:A:1681:PHE:HD1	2:A:1687:SER:HG	1.53	0.54
2:A:1707:ILE:HD13	2:A:1740:PHE:CE2	2.42	0.54
1:C:59:ASN:HB3	1:C:62:GLN:CB	2.34	0.54
2:A:207:LEU:HD11	2:A:209:ASN:CG	2.33	0.54
2:A:806:VAL:CG2	2:A:809:ASN:CB	2.85	0.54
2:A:131:LEU:HD22	2:A:131:LEU:C	2.33	0.54
2:A:184:LEU:CD1	2:A:190:TRP:CD1	2.91	0.54
2:A:790:GLU:O	2:A:794:LYS:N	2.38	0.54
2:A:798:MET:O	2:A:799:ASP:HB2	2.07	0.54
2:A:895:CYS:HB2	2:A:938:VAL:CG1	2.38	0.54
3:B:90:VAL:HG11	3:B:106:ILE:HD11	1.90	0.54
3:B:180:TYR:CD1	3:B:180:TYR:C	2.85	0.54
1:C:52:PHE:CD1	1:C:52:PHE:C	2.85	0.54
2:A:399:ALA:HB3	2:A:1762:ASN:HD22	1.63	0.54
2:A:1509:PHE:CD1	2:A:1509:PHE:C	2.85	0.54
2:A:183:PHE:C	2:A:183:PHE:CD1	2.85	0.54
2:A:803:TYR:CE1	2:A:809:ASN:ND2	2.68	0.54
3:B:182:TYR:CD1	3:B:182:TYR:C	2.85	0.54
2:A:217:ARG:CZ	2:A:217:ARG:CB	2.85	0.54
3:B:26:SER:HB2	3:B:39:LEU:H	1.71	0.54
1:C:33:THR:O	1:C:50:CYS:CA	2.55	0.54
2:A:196:ILE:CD1	2:A:197:VAL:N	2.70	0.54
2:A:911:ASN:HD22	2:A:911:ASN:C	2.12	0.54
2:A:146:ASN:O	2:A:147:ASN:HB3	2.09	0.53
2:A:1186:TYR:CZ	2:A:1190:GLU:OE2	2.62	0.53
1:C:62:GLN:HB3	1:C:132:PRO:HD2	1.90	0.53
2:A:810:ILE:O	2:A:814:LEU:CD1	2.43	0.53
2:A:1477:GLU:OE2	2:A:1477:GLU:HA	2.07	0.53
2:A:1535:GLU:HG2	2:A:1547:LEU:CD1	2.39	0.53
2:A:1573:TYR:CD1	2:A:1573:TYR:C	2.85	0.53
3:B:119:TYR:O	3:B:142:ILE:N	2.39	0.53
2:A:867:GLY:O	2:A:870:THR:HG23	2.09	0.53
2:A:900:ASN:OD1	2:A:902:ASP:N	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:71:LEU:CD2	3:B:106:ILE:HD11	2.37	0.53
4:E:2:NAG:HO3	4:E:2:NAG:C7	2.13	0.53
1:C:135:ARG:HH21	1:C:135:ARG:CG	2.14	0.53
2:A:187:PRO:HA	2:A:190:TRP:CE3	2.44	0.53
2:A:741:VAL:HG23	2:A:742:MET:N	2.22	0.53
2:A:1732:ASN:OD1	2:A:1735:VAL:HB	2.08	0.53
2:A:1760:LEU:HD23	2:A:1760:LEU:C	2.33	0.53
2:A:1495:LYS:CE	2:A:1495:LYS:HA	2.38	0.53
3:B:89:ARG:NH1	3:B:110:ASN:OD1	2.42	0.53
2:A:936:MET:HE3	2:A:945:LEU:HG	1.90	0.53
2:A:1298:LEU:HD12	2:A:1301:LEU:HD12	1.89	0.53
2:A:1517:PHE:CD1	2:A:1517:PHE:C	2.85	0.53
1:C:107:LYS:O	1:C:107:LYS:HG2	2.08	0.53
2:A:772:PHE:HD1	2:A:772:PHE:O	1.92	0.53
3:B:178:MET:O	3:B:182:TYR:HB3	2.08	0.53
2:A:114:PRO:O	2:A:118:ILE:HG12	2.09	0.53
2:A:175:GLY:O	2:A:178:VAL:HB	2.09	0.53
2:A:293:LEU:CD1	2:A:298:ASP:C	2.81	0.53
2:A:1408:TRP:CD1	2:A:1409:THR:H	2.27	0.52
2:A:963:PHE:CD1	2:A:963:PHE:C	2.87	0.52
2:A:1532:MET:CE	2:A:1616:ARG:HB2	2.39	0.52
2:A:176:PHE:O	2:A:178:VAL:HG23	2.08	0.52
2:A:1365:PRO:O	2:A:1424:GLN:CB	2.57	0.52
2:A:1408:TRP:CD1	2:A:1409:THR:N	2.77	0.52
2:A:165:PHE:O	2:A:169:VAL:HG13	2.09	0.52
1:C:32:VAL:CG1	1:C:50:CYS:SG	2.98	0.52
2:A:207:LEU:CD1	2:A:209:ASN:N	2.73	0.52
2:A:279:SER:C	2:A:280:LEU:HD12	2.34	0.52
2:A:300:ARG:NH1	3:B:130:GLU:OE2	2.43	0.52
2:A:734:LYS:CE	2:A:799:ASP:OD2	2.58	0.52
2:A:1495:LYS:CA	2:A:1495:LYS:HE3	2.39	0.52
2:A:849:TRP:HH2	2:A:1326:LEU:HB3	1.74	0.52
2:A:1757:ALA:O	2:A:1761:GLU:HG2	2.09	0.52
3:B:57:TRP:CH2	3:B:142:ILE:HD13	2.40	0.52
2:A:114:PRO:HG2	2:A:115:LEU:H	1.74	0.52
2:A:262:ILE:CG1	2:A:1617:ILE:CD1	2.88	0.52
2:A:397:ILE:O	2:A:401:VAL:HG23	2.09	0.52
2:A:1293:ARG:O	2:A:1295:LEU:N	2.42	0.52
2:A:890:LYS:NZ	2:A:890:LYS:CB	2.73	0.52
2:A:1512:VAL:CG1	2:A:1565:LYS:HG3	2.39	0.52
2:A:1752:VAL:O	2:A:1756:ILE:HG12	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:159:PHE:O	2:A:163:TYR:CD2	2.62	0.52
2:A:338:ASP:O	2:A:339:TYR:HB2	2.10	0.52
2:A:1294:ALA:O	2:A:1297:PRO:CD	2.57	0.52
2:A:1308:ARG:CB	2:A:1308:ARG:NH2	2.73	0.52
2:A:1349:GLU:HG3	2:A:1351:ILE:CG2	2.40	0.52
2:A:1733:PRO:O	2:A:1737:ILE:HG13	2.10	0.52
2:A:217:ARG:CG	2:A:217:ARG:HH11	2.22	0.52
2:A:224:THR:HA	2:A:227:VAL:CG2	2.40	0.51
2:A:329:THR:CG2	2:A:330:CYS:N	2.71	0.51
2:A:838:ARG:NH1	2:A:838:ARG:CG	2.73	0.51
2:A:279:SER:O	2:A:280:LEU:HD12	2.10	0.51
2:A:290:MET:HG3	2:A:333:ILE:HG21	1.92	0.51
2:A:791:MET:HE3	2:A:795:LEU:CD2	2.38	0.51
2:A:1495:LYS:CE	2:A:1495:LYS:CA	2.86	0.51
3:B:60:ARG:HD2	3:B:60:ARG:O	2.09	0.51
3:B:66:GLU:C	3:B:67:PHE:CD1	2.88	0.51
1:C:47:ARG:NH2	1:C:111:SER:OG	2.43	0.51
2:A:293:LEU:CD1	2:A:298:ASP:CB	2.56	0.51
2:A:300:ARG:HH11	2:A:300:ARG:CG	2.18	0.51
2:A:810:ILE:HG13	2:A:811:PHE:H	1.75	0.51
2:A:1408:TRP:NE1	2:A:1409:THR:HG22	2.25	0.51
2:A:1509:PHE:N	2:A:1568:SER:OG	2.43	0.51
3:B:85:ARG:HG2	3:B:85:ARG:NH1	2.18	0.51
2:A:1408:TRP:NE1	2:A:1409:THR:CG2	2.73	0.51
2:A:1707:ILE:HD13	2:A:1740:PHE:HE2	1.74	0.51
3:B:58:THR:HG22	3:B:69:LYS:CA	2.39	0.51
2:A:204:PHE:O	2:A:205:VAL:C	2.53	0.51
2:A:798:MET:HE2	2:A:803:TYR:HD1	1.72	0.51
2:A:831:LEU:N	2:A:831:LEU:CD2	2.73	0.51
2:A:1281:SER:O	2:A:1282:ASP:HB2	2.10	0.51
2:A:1499:ARG:HG2	2:A:1509:PHE:CD1	2.45	0.51
2:A:1509:PHE:CA	2:A:1568:SER:HB3	2.40	0.51
2:A:144:THR:O	2:A:144:THR:HG22	2.09	0.51
2:A:207:LEU:HD12	2:A:213:LEU:CG	2.41	0.51
2:A:1680:ASN:O	2:A:1686:ASN:HB3	2.11	0.51
2:A:415:GLU:OE2	2:A:416:ALA:HB2	2.09	0.51
2:A:840:LEU:C	2:A:842:VAL:H	2.18	0.51
2:A:896:VAL:CG1	2:A:905:LEU:HD13	2.41	0.51
2:A:1190:GLU:HA	2:A:1190:GLU:OE1	2.11	0.51
2:A:1340:VAL:O	2:A:1344:ALA:HB2	2.11	0.51
2:A:117:ARG:CG	2:A:117:ARG:NH1	2.73	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:147:ASN:HD22	2:A:147:ASN:C	2.18	0.51
2:A:798:MET:HE2	2:A:803:TYR:HA	1.91	0.51
2:A:852:LEU:CD1	2:A:1327:VAL:HG13	2.40	0.51
2:A:1293:ARG:HH21	2:A:1293:ARG:HB3	1.75	0.51
2:A:1522:MET:HE1	2:A:1623:LEU:HD22	1.81	0.51
2:A:133:MET:SD	2:A:133:MET:C	2.94	0.51
2:A:278:ASN:HD21	2:A:329:THR:HB	1.76	0.50
2:A:740:ILE:O	2:A:740:ILE:HG22	2.10	0.50
2:A:1218:ARG:CG	2:A:1218:ARG:NH2	2.73	0.50
2:A:1301:LEU:HD23	2:A:1307:MET:HG2	1.93	0.50
2:A:1304:PHE:HB2	2:A:1307:MET:HE2	1.92	0.50
2:A:1527:LEU:O	2:A:1530:VAL:HG12	2.11	0.50
2:A:761:MET:CE	2:A:839:LEU:HB3	2.41	0.50
2:A:803:TYR:CZ	2:A:809:ASN:ND2	2.74	0.50
2:A:901:ASP:OD1	2:A:901:ASP:N	2.44	0.50
2:A:1460:PHE:HD2	2:A:1756:ILE:HG13	1.76	0.50
2:A:1527:LEU:O	2:A:1530:VAL:CG1	2.58	0.50
2:A:1606:PRO:O	2:A:1609:PHE:HB3	2.11	0.50
1:C:128:TYR:HB3	1:C:137:ARG:HE	1.77	0.50
2:A:164:THR:O	2:A:168:LEU:N	2.35	0.50
2:A:762:ALA:O	2:A:1392:VAL:CG2	2.60	0.50
2:A:971:PHE:CD1	2:A:971:PHE:C	2.88	0.50
3:B:112:THR:CG2	3:B:113:TYR:N	2.74	0.50
2:A:272:LYS:NZ	2:A:345:ASP:OD2	2.44	0.50
2:A:762:ALA:O	2:A:1392:VAL:HG21	2.11	0.50
3:B:104:LEU:N	3:B:104:LEU:CD2	2.73	0.50
2:A:329:THR:HG23	2:A:330:CYS:N	2.27	0.50
2:A:739:PHE:O	2:A:742:MET:HE2	2.12	0.50
3:B:129:PHE:HB2	3:B:132:TYR:O	2.12	0.50
2:A:207:LEU:HD11	2:A:209:ASN:H	1.76	0.50
2:A:336:ASN:HB2	2:A:343:SER:OG	2.11	0.50
2:A:1215:TYR:HD1	2:A:1218:ARG:HD3	1.76	0.50
2:A:1573:TYR:OH	2:A:1583:PHE:HB2	2.11	0.50
2:A:326:GLU:HG3	3:B:45:ARG:HG3	1.93	0.50
2:A:1514:ASN:ND2	2:A:1515:GLN:N	2.60	0.50
1:C:34:VAL:HG21	1:C:142:ILE:HG13	1.93	0.50
2:A:1273:LEU:HD12	2:A:1273:LEU:C	2.36	0.50
2:A:1511:LEU:C	2:A:1511:LEU:CD2	2.85	0.50
2:A:1628:LYS:CD	2:A:1628:LYS:C	2.85	0.50
3:B:85:ARG:CG	3:B:85:ARG:NH1	2.73	0.50
2:A:321:SER:CB	2:A:375:GLY:HA2	2.34	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:112:THR:HG22	3:B:113:TYR:H	1.74	0.50
2:A:1282:ASP:HA	2:A:1287:LYS:HB2	1.94	0.49
2:A:1360:PRO:O	2:A:1361:ALA:HB3	2.12	0.49
2:A:1514:ASN:HD22	2:A:1515:GLN:H	1.60	0.49
2:A:1293:ARG:C	2:A:1295:LEU:N	2.70	0.49
3:B:38:ILE:CG2	3:B:142:ILE:HD13	2.42	0.49
2:A:123:LEU:C	2:A:123:LEU:CD2	2.86	0.49
2:A:1369:GLU:OE1	2:A:1369:GLU:HA	2.12	0.49
2:A:1412:MET:HE3	2:A:1434:TYR:CD1	2.48	0.49
2:A:1491:LYS:C	2:A:1491:LYS:CD	2.86	0.49
2:A:1502:ASN:HB3	2:A:1504:ILE:HD13	1.89	0.49
2:A:1635:PHE:CD1	2:A:1638:MET:HE2	2.47	0.49
1:C:34:VAL:HG21	1:C:142:ILE:CG1	2.42	0.49
2:A:151:TRP:CE3	2:A:152:THR:HA	2.47	0.49
3:B:141:LYS:HZ2	3:B:141:LYS:HB3	1.76	0.49
3:B:144:ILE:O	3:B:144:ILE:HG13	2.12	0.49
2:A:147:ASN:C	2:A:147:ASN:ND2	2.70	0.49
2:A:332:LYS:C	2:A:333:ILE:HG12	2.37	0.49
2:A:798:MET:HE3	2:A:803:TYR:CA	2.24	0.49
2:A:879:ILE:O	2:A:882:VAL:HG12	2.13	0.49
2:A:1287:LYS:HE3	2:A:1287:LYS:O	2.12	0.49
2:A:279:SER:C	2:A:280:LEU:CD1	2.86	0.49
2:A:361:ASP:OD2	2:A:929:ILE:CG2	2.60	0.49
2:A:899:ILE:CG2	2:A:938:VAL:HG13	2.43	0.49
2:A:1205:SER:O	2:A:1296:ARG:NH1	2.46	0.49
2:A:1496:PRO:C	2:A:1497:ILE:CG1	2.85	0.49
2:A:1640:SER:CB	2:A:1761:GLU:HG3	2.42	0.49
1:C:54:SER:HB2	1:C:134:ASP:OD2	2.13	0.49
2:A:117:ARG:O	2:A:120:ILE:HG22	2.12	0.49
2:A:758:THR:HG23	2:A:759:LEU:N	2.28	0.49
2:A:793:LEU:C	2:A:793:LEU:CD1	2.86	0.49
2:A:1220:LYS:NZ	3:B:27:GLU:OE2	2.46	0.49
1:C:128:TYR:CE2	1:C:137:ARG:NH2	2.74	0.49
2:A:1270:LEU:C	2:A:1270:LEU:CD1	2.85	0.49
1:C:61:LYS:CG	1:C:85:MET:HE1	2.32	0.49
2:A:125:HIS:ND1	2:A:126:SER:N	2.60	0.49
2:A:945:LEU:CD2	2:A:949:MET:HE3	2.43	0.49
3:B:54:PHE:CE1	3:B:124:TYR:CD2	2.87	0.49
3:B:89:ARG:O	3:B:108:ILE:HA	2.13	0.49
3:B:126:LEU:HD13	3:B:128:PHE:CE1	2.46	0.49
2:A:291:ASN:ND2	2:A:292:THR:N	2.60	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:750:ILE:O	2:A:753:CYS:HB3	2.12	0.49
2:A:1293:ARG:CB	2:A:1293:ARG:NH2	2.73	0.49
2:A:1532:MET:HG3	2:A:1616:ARG:HH12	1.77	0.49
1:C:34:VAL:CG2	1:C:142:ILE:CG1	2.91	0.48
2:A:191:LEU:C	2:A:191:LEU:CD2	2.85	0.48
2:A:1218:ARG:CZ	2:A:1218:ARG:CB	2.91	0.48
2:A:1509:PHE:CA	2:A:1568:SER:CB	2.92	0.48
2:A:1667:ALA:O	2:A:1668:TYR:HB2	2.13	0.48
2:A:145:MET:CA	2:A:145:MET:CE	2.85	0.48
2:A:349:TRP:HA	2:A:349:TRP:HE3	1.78	0.48
2:A:823:LEU:C	2:A:823:LEU:CD2	2.85	0.48
2:A:833:VAL:HG13	2:A:834:LEU:N	2.28	0.48
2:A:842:VAL:O	2:A:845:LEU:HG	2.13	0.48
2:A:890:LYS:HZ3	2:A:890:LYS:HB3	1.76	0.48
2:A:1287:LYS:C	2:A:1287:LYS:CD	2.85	0.48
2:A:1321:ILE:CD1	2:A:1456:ILE:HG12	2.42	0.48
2:A:1574:PHE:CD1	2:A:1580:ILE:HD11	2.36	0.48
2:A:116:ARG:NH2	2:A:176:PHE:HB2	2.28	0.48
2:A:928:TRP:HZ3	2:A:932:MET:HE1	1.78	0.48
1:C:55:CYS:C	1:C:56:TYR:CG	2.90	0.48
2:A:772:PHE:CD1	2:A:772:PHE:C	2.91	0.48
2:A:1760:LEU:C	2:A:1760:LEU:CD2	2.86	0.48
1:C:34:VAL:HG23	1:C:35:PRO:N	2.29	0.48
2:A:136:ILE:CD1	2:A:136:ILE:C	2.85	0.48
2:A:339:TYR:HB2	2:A:341:TYR:CD2	2.49	0.48
2:A:803:TYR:CE2	2:A:809:ASN:OD1	2.67	0.48
2:A:1318:ILE:HG13	2:A:1319:PRO:N	2.28	0.48
2:A:1407:GLY:N	6:A:2007:9SL:O01	2.47	0.48
2:A:1497:ILE:HG22	2:A:1498:PRO:CD	2.44	0.48
2:A:291:ASN:HD22	2:A:291:ASN:C	2.21	0.48
2:A:1254:PHE:HD1	2:A:1260:TRP:CE2	2.32	0.48
2:A:1373:LEU:O	2:A:1377:SER:HB2	2.13	0.48
2:A:1408:TRP:CD1	2:A:1409:THR:CG2	2.97	0.48
2:A:1677:ASP:CG	3:B:46:ARG:NH1	2.72	0.48
3:B:174:LEU:O	3:B:178:MET:HG2	2.13	0.48
2:A:284:GLU:HB3	2:A:289:ILE:HD11	1.95	0.48
1:C:61:LYS:HA	1:C:85:MET:SD	2.54	0.48
1:C:107:LYS:CD	1:C:109:ASP:HB2	2.41	0.48
2:A:286:LEU:HD11	2:A:333:ILE:HG13	1.96	0.48
2:A:327:GLY:HA3	3:B:134:HIS:CD2	2.48	0.48
2:A:733:PHE:O	2:A:737:ILE:HG12	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1503:LYS:CD	2:A:1503:LYS:N	2.73	0.48
2:A:1191:HIS:ND1	2:A:1192:SER:N	2.61	0.48
2:A:1532:MET:SD	2:A:1620:ILE:CD1	2.98	0.48
2:A:1641:LEU:HD23	2:A:1641:LEU:HA	1.73	0.48
3:B:53:THR:CG2	3:B:54:PHE:N	2.77	0.48
2:A:322:GLY:HA3	2:A:323:GLN:HG2	1.95	0.47
2:A:1301:LEU:HD22	2:A:1311:VAL:HG21	1.95	0.47
2:A:116:ARG:HH22	2:A:176:PHE:HB2	1.79	0.47
2:A:217:ARG:NH1	2:A:217:ARG:CB	2.75	0.47
2:A:273:HIS:O	2:A:314:LEU:HD12	2.13	0.47
2:A:843:PHE:C	2:A:845:LEU:N	2.70	0.47
2:A:1503:LYS:H	2:A:1503:LYS:HD3	1.78	0.47
2:A:1710:SER:O	2:A:1711:LYS:HG2	2.14	0.47
2:A:783:PHE:O	2:A:787:PHE:CD2	2.65	0.47
2:A:869:LEU:HD12	2:A:869:LEU:C	2.32	0.47
2:A:1555:ILE:HD12	2:A:1593:MET:HE3	1.95	0.47
2:A:1650:LEU:C	2:A:1650:LEU:CD1	2.86	0.47
2:A:764:GLU:C	2:A:765:HIS:ND1	2.73	0.47
3:B:88:GLY:O	3:B:89:ARG:HB2	2.14	0.47
2:A:196:ILE:O	2:A:200:TYR:CD1	2.65	0.47
2:A:247:ASP:OD2	2:A:1629:GLY:HA3	2.15	0.47
2:A:1242:LEU:O	2:A:1246:ILE:HG12	2.15	0.47
2:A:1460:PHE:CE2	2:A:1753:ASN:ND2	2.82	0.47
2:A:1509:PHE:HB2	2:A:1568:SER:CB	2.31	0.47
2:A:1574:PHE:CD1	2:A:1580:ILE:CD1	2.91	0.47
2:A:116:ARG:CZ	2:A:176:PHE:HB2	2.44	0.47
2:A:191:LEU:HD23	2:A:191:LEU:C	2.39	0.47
2:A:248:VAL:CG2	2:A:400:VAL:HG21	2.44	0.47
2:A:415:GLU:CD	2:A:416:ALA:N	2.73	0.47
2:A:1459:ASN:O	2:A:1459:ASN:ND2	2.48	0.47
2:A:1635:PHE:CD1	2:A:1638:MET:CE	2.97	0.47
2:A:1719:LYS:H	2:A:1728:GLY:N	2.13	0.47
3:B:55:THR:CG2	3:B:56:GLU:N	2.77	0.47
2:A:285:THR:O	2:A:289:ILE:HG12	2.15	0.47
2:A:1179:TRP:HE1	2:A:1183:LYS:HE2	1.80	0.47
2:A:1318:ILE:HG12	2:A:1319:PRO:HD3	1.96	0.47
3:B:101:LEU:O	3:B:103:ASP:N	2.43	0.47
4:E:1:NAG:H82	4:E:1:NAG:C1	2.44	0.47
2:A:361:ASP:OD2	2:A:929:ILE:CB	2.63	0.47
2:A:738:TYR:CD1	2:A:738:TYR:C	2.93	0.47
2:A:890:LYS:CB	2:A:890:LYS:HZ3	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:945:LEU:HD23	2:A:949:MET:CE	2.45	0.47
2:A:1638:MET:HE3	2:A:1639:MET:HE3	1.97	0.47
2:A:259:PHE:HB2	2:A:354:LEU:HD22	1.97	0.47
2:A:1502:ASN:CB	2:A:1504:ILE:HD11	2.20	0.47
2:A:114:PRO:CG	2:A:115:LEU:H	2.27	0.46
2:A:259:PHE:HB3	2:A:354:LEU:HD21	1.97	0.46
2:A:276:PHE:CE2	2:A:280:LEU:HD21	2.47	0.46
2:A:795:LEU:HD13	2:A:803:TYR:CE2	2.49	0.46
2:A:1366:ASN:OD1	2:A:1366:ASN:N	2.46	0.46
2:A:1419:VAL:HG12	2:A:1425:PRO:HA	1.96	0.46
2:A:171:ILE:HD12	2:A:172:LEU:N	2.30	0.46
2:A:321:SER:OG	2:A:322:GLY:N	2.48	0.46
2:A:954:ILE:O	2:A:958:VAL:HG23	2.16	0.46
2:A:1420:ASN:HB3	2:A:1423:LYS:HG3	1.97	0.46
3:B:51:ALA:CB	3:B:127:LEU:HA	2.44	0.46
2:A:219:LEU:O	2:A:222:LEU:HB2	2.14	0.46
2:A:1522:MET:CA	2:A:1522:MET:HE3	2.45	0.46
2:A:333:ILE:HG22	2:A:334:GLY:N	2.30	0.46
2:A:960:LEU:HD23	2:A:960:LEU:C	2.41	0.46
2:A:1509:PHE:HA	2:A:1568:SER:HB3	1.95	0.46
2:A:1623:LEU:HD23	2:A:1623:LEU:HA	1.75	0.46
2:A:132:ILE:CD1	2:A:166:GLU:HB3	2.23	0.46
2:A:176:PHE:HD2	2:A:178:VAL:HG21	1.80	0.46
2:A:217:ARG:HG2	2:A:217:ARG:HH11	1.80	0.46
2:A:315:CYS:CB	2:A:324:CYS:SG	3.00	0.46
2:A:399:ALA:O	2:A:403:MET:HB2	2.14	0.46
2:A:825:LEU:HD22	2:A:825:LEU:HA	1.79	0.46
2:A:1218:ARG:HB3	2:A:1218:ARG:CZ	2.45	0.46
2:A:1508:ILE:CG2	2:A:1564:LEU:CD1	2.93	0.46
2:A:1709:ASN:HB2	2:A:1714:ASP:CB	2.41	0.46
1:C:34:VAL:CG1	1:C:50:CYS:SG	2.96	0.46
2:A:1459:ASN:ND2	2:A:1459:ASN:C	2.73	0.46
3:B:50:ASN:ND2	3:B:50:ASN:C	2.73	0.46
2:A:398:LEU:HD12	2:A:960:LEU:HD11	1.97	0.46
2:A:909:HIS:HD2	2:A:911:ASN:N	2.07	0.46
2:A:1349:GLU:HG3	2:A:1351:ILE:HG22	1.98	0.46
2:A:1497:ILE:HG22	2:A:1498:PRO:HD2	1.97	0.46
2:A:1571:HIS:CD2	2:A:1571:HIS:H	2.33	0.46
2:A:206:ASN:OD1	2:A:206:ASN:N	2.48	0.46
2:A:218:VAL:CG1	2:A:879:ILE:HG23	2.46	0.46
2:A:291:ASN:ND2	2:A:291:ASN:C	2.74	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:388:LEU:O	2:A:388:LEU:HD13	2.15	0.46
2:A:395:ASN:ND2	2:A:1755:TYR:CD1	2.83	0.46
2:A:214:ARG:HA	2:A:214:ARG:HD3	1.61	0.46
2:A:741:VAL:CG2	2:A:742:MET:N	2.78	0.46
2:A:854:MET:O	2:A:858:ILE:HG13	2.16	0.46
2:A:931:THR:HG22	2:A:948:TYR:OH	2.16	0.46
3:B:46:ARG:NH2	3:B:48:GLU:CD	2.73	0.46
3:B:54:PHE:CD2	3:B:124:TYR:HB2	2.51	0.46
2:A:772:PHE:HD1	2:A:772:PHE:C	2.24	0.46
2:A:964:LEU:HD13	2:A:964:LEU:HA	1.80	0.46
2:A:1308:ARG:NH2	2:A:1308:ARG:HB3	2.30	0.46
3:B:75:ASN:CG	3:B:76:GLU:N	2.74	0.46
3:B:154:MET:O	3:B:158:VAL:HG23	2.16	0.46
1:C:103:GLY:C	1:C:105:PRO:HD3	2.40	0.45
2:A:136:ILE:HG23	2:A:137:LEU:N	2.30	0.45
2:A:902:ASP:HB3	2:A:904:THR:HG22	1.97	0.45
2:A:1194:PHE:CD1	2:A:1194:PHE:C	2.94	0.45
2:A:361:ASP:OD2	2:A:929:ILE:HB	2.15	0.45
2:A:757:ASN:ND2	2:A:757:ASN:C	2.73	0.45
2:A:788:ALA:HA	2:A:816:VAL:HG11	1.97	0.45
2:A:1179:TRP:CD1	2:A:1183:LYS:CE	2.99	0.45
2:A:1325:LEU:HD12	2:A:1329:LEU:HG	1.99	0.45
2:A:1548:TYR:CD1	2:A:1548:TYR:C	2.94	0.45
3:B:50:ASN:C	3:B:50:ASN:HD22	2.24	0.45
3:B:54:PHE:CE2	3:B:124:TYR:CB	2.96	0.45
2:A:116:ARG:NH1	2:A:176:PHE:HA	2.29	0.45
2:A:336:ASN:HD22	2:A:343:SER:CB	2.21	0.45
2:A:772:PHE:O	2:A:772:PHE:CD1	2.70	0.45
2:A:1212:GLU:O	2:A:1213:ASP:CB	2.64	0.45
2:A:1280:TYR:O	2:A:1283:LEU:HD21	2.17	0.45
3:B:67:PHE:CD2	3:B:120:GLU:HG3	2.49	0.45
2:A:132:ILE:CD1	2:A:166:GLU:CG	2.94	0.45
2:A:196:ILE:C	2:A:196:ILE:CD1	2.85	0.45
2:A:276:PHE:N	2:A:329:THR:O	2.46	0.45
2:A:1404:THR:O	2:A:1405:PHE:HB2	2.15	0.45
2:A:169:VAL:HG23	2:A:170:LYS:N	2.31	0.45
2:A:248:VAL:HG21	2:A:400:VAL:HG21	1.98	0.45
2:A:314:LEU:HD12	2:A:314:LEU:HA	1.86	0.45
2:A:956:ASN:N	2:A:956:ASN:HD22	2.14	0.45
2:A:1508:ILE:HG21	2:A:1564:LEU:CD1	2.46	0.45
2:A:147:ASN:HD22	2:A:147:ASN:N	2.13	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:217:ARG:CG	2:A:217:ARG:NH1	2.79	0.45
2:A:846:ALA:HA	2:A:852:LEU:HD23	1.99	0.45
2:A:1273:LEU:O	2:A:1277:THR:OG1	2.34	0.45
2:A:1295:LEU:CD1	2:A:1298:LEU:CD2	2.86	0.45
2:A:1364:VAL:CG2	2:A:1370:CYS:HA	2.46	0.45
3:B:38:ILE:HB	3:B:106:ILE:HG22	1.99	0.45
3:B:128:PHE:CD1	3:B:128:PHE:N	2.84	0.45
2:A:759:LEU:HD22	2:A:759:LEU:HA	1.74	0.45
2:A:1405:PHE:HE1	2:A:1441:ILE:HD13	1.81	0.45
2:A:1607:THR:HG23	2:A:1610:ARG:NH1	2.25	0.45
2:A:754:ILE:HG12	2:A:787:PHE:HE1	1.77	0.45
2:A:1444:GLY:O	2:A:1448:THR:OG1	2.32	0.45
2:A:1497:ILE:HG12	2:A:1572:TYR:HB3	1.98	0.45
2:A:1681:PHE:HD1	2:A:1687:SER:OG	1.99	0.45
2:A:766:HIS:CD2	2:A:766:HIS:O	2.70	0.45
2:A:1343:PHE:HB3	2:A:1347:PHE:CE1	2.51	0.45
2:A:1355:ASP:OD1	2:A:1355:ASP:N	2.50	0.45
2:A:1412:MET:HE3	2:A:1434:TYR:HD1	1.80	0.45
2:A:1710:SER:O	2:A:1711:LYS:HE3	2.17	0.45
1:C:55:CYS:O	1:C:56:TYR:CD2	2.70	0.44
2:A:163:TYR:O	2:A:166:GLU:HG3	2.17	0.44
2:A:176:PHE:O	2:A:176:PHE:CG	2.70	0.44
2:A:371:LEU:O	2:A:375:GLY:N	2.44	0.44
2:A:1528:ASN:C	2:A:1528:ASN:ND2	2.73	0.44
2:A:1530:VAL:HA	2:A:1533:MET:HG3	1.99	0.44
2:A:1719:LYS:H	2:A:1728:GLY:H	1.65	0.44
2:A:280:LEU:CD1	2:A:280:LEU:N	2.80	0.44
1:C:131:ASN:O	1:C:134:ASP:N	2.51	0.44
2:A:300:ARG:NH1	2:A:300:ARG:CG	2.75	0.44
2:A:388:LEU:C	2:A:388:LEU:CD1	2.85	0.44
2:A:794:LYS:CG	2:A:803:TYR:CE1	2.75	0.44
2:A:1491:LYS:HD3	2:A:1491:LYS:C	2.43	0.44
2:A:1611:VAL:O	2:A:1614:LEU:HB2	2.17	0.44
1:C:55:CYS:O	1:C:56:TYR:CG	2.69	0.44
2:A:121:LYS:HB2	2:A:121:LYS:HE3	1.58	0.44
2:A:197:VAL:O	2:A:201:LEU:HB2	2.18	0.44
2:A:231:LEU:HD12	2:A:231:LEU:HA	1.73	0.44
2:A:290:MET:HE2	2:A:333:ILE:CG2	2.45	0.44
2:A:834:LEU:O	2:A:837:PHE:CB	2.60	0.44
2:A:1298:LEU:HD12	2:A:1301:LEU:CD1	2.48	0.44
2:A:1691:LEU:HD13	2:A:1743:TYR:CE2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:743:ASP:N	2:A:744:PRO:HD2	2.32	0.44
2:A:1281:SER:OG	2:A:1282:ASP:OD1	2.32	0.44
2:A:1364:VAL:HG23	2:A:1370:CYS:CA	2.47	0.44
2:A:1569:LEU:HB2	2:A:1573:TYR:HB2	2.00	0.44
2:A:410:GLN:C	2:A:413:ILE:HG22	2.43	0.44
2:A:738:TYR:O	2:A:738:TYR:CD1	2.70	0.44
2:A:1280:TYR:O	2:A:1280:TYR:CD1	2.70	0.44
2:A:1280:TYR:O	2:A:1280:TYR:HD1	2.00	0.44
2:A:1292:LEU:HD12	2:A:1292:LEU:HA	1.78	0.44
2:A:1338:MET:HE3	2:A:1338:MET:HB2	1.81	0.44
3:B:119:TYR:N	3:B:142:ILE:O	2.46	0.44
1:C:41:LEU:HD21	1:C:147:LEU:HD22	2.00	0.44
2:A:234:ILE:HG13	2:A:868:ASN:HB3	2.00	0.44
2:A:971:PHE:HD1	2:A:972:SER:HB2	1.83	0.44
1:C:61:LYS:HG3	1:C:85:MET:SD	2.58	0.44
2:A:867:GLY:HA2	2:A:870:THR:HG22	2.00	0.44
2:A:896:VAL:HG12	2:A:905:LEU:HD13	2.00	0.44
2:A:1495:LYS:HE3	2:A:1495:LYS:N	2.33	0.44
3:B:88:GLY:O	3:B:89:ARG:CB	2.65	0.44
2:A:286:LEU:HD22	2:A:286:LEU:C	2.43	0.44
2:A:1670:LYS:HB3	2:A:1670:LYS:HE3	1.71	0.44
3:B:117:GLY:O	3:B:143:HIS:HD2	2.00	0.44
2:A:139:ASN:O	2:A:139:ASN:ND2	2.39	0.43
2:A:283:ASN:HB2	5:A:2006:NAG:H2	1.99	0.43
2:A:327:GLY:CA	3:B:134:HIS:CD2	3.01	0.43
2:A:410:GLN:HA	2:A:413:ILE:HG22	1.99	0.43
2:A:757:ASN:ND2	2:A:757:ASN:O	2.51	0.43
2:A:765:HIS:HA	2:A:1390:ASP:O	2.17	0.43
2:A:789:ALA:HA	2:A:792:VAL:HG12	2.00	0.43
2:A:1293:ARG:C	2:A:1295:LEU:H	2.26	0.43
2:A:1407:GLY:CA	6:A:2007:9SL:O01	2.66	0.43
2:A:144:THR:HG23	2:A:913:PHE:CB	2.48	0.43
2:A:730:TRP:O	2:A:734:LYS:N	2.43	0.43
2:A:118:ILE:N	2:A:118:ILE:CD1	2.73	0.43
2:A:171:ILE:C	2:A:171:ILE:CD1	2.86	0.43
2:A:769:THR:HG23	2:A:772:PHE:HB2	1.99	0.43
2:A:791:MET:HB3	2:A:791:MET:HE2	1.67	0.43
2:A:1317:ALA:CB	2:A:1459:ASN:OD1	2.66	0.43
2:A:1506:GLY:O	2:A:1510:ASP:N	2.44	0.43
3:B:101:LEU:N	3:B:101:LEU:HD13	2.33	0.43
1:C:56:TYR:HD1	2:A:898:LYS:HD2	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:782:VAL:O	2:A:786:ILE:HG12	2.17	0.43
2:A:899:ILE:HG23	2:A:938:VAL:HG13	1.99	0.43
2:A:1437:PHE:O	2:A:1441:ILE:HG13	2.17	0.43
3:B:51:ALA:HB3	3:B:127:LEU:CD1	2.41	0.43
3:B:57:TRP:HH2	3:B:142:ILE:HD13	1.78	0.43
2:A:882:VAL:O	2:A:886:GLN:HG2	2.18	0.43
2:A:1613:ARG:C	2:A:1615:ALA:N	2.74	0.43
2:A:196:ILE:HD12	2:A:197:VAL:CA	2.48	0.43
2:A:923:VAL:HG13	2:A:928:TRP:HB3	1.99	0.43
2:A:1675:ILE:HD12	2:A:1706:PRO:HG3	2.01	0.43
1:C:135:ARG:NH2	1:C:135:ARG:CG	2.73	0.43
2:A:140:CYS:HA	2:A:143:MET:HG3	2.00	0.43
2:A:737:ILE:O	2:A:740:ILE:HB	2.19	0.43
2:A:1189:VAL:HG11	2:A:1244:LYS:HD3	2.00	0.43
2:A:1321:ILE:CD1	2:A:1456:ILE:CG1	2.97	0.43
1:C:30:MET:HE3	1:C:30:MET:HB3	1.66	0.43
2:A:131:LEU:C	2:A:131:LEU:CD1	2.85	0.43
2:A:967:LEU:CD2	2:A:967:LEU:C	2.85	0.43
2:A:1232:ILE:HD11	3:B:166:LEU:HB3	2.01	0.43
2:A:1457:ILE:HD12	2:A:1458:ASP:CA	2.48	0.43
2:A:1764:SER:HA	2:A:1767:THR:HG22	2.01	0.43
1:C:108:TYR:N	1:C:108:TYR:CD1	2.86	0.43
2:A:168:LEU:HD23	2:A:169:VAL:CA	2.49	0.43
2:A:1218:ARG:NH2	2:A:1218:ARG:CB	2.82	0.43
2:A:1430:SER:HB3	2:A:1433:MET:CG	2.46	0.43
2:A:1467:LEU:HD21	2:A:1472:ILE:HG22	2.00	0.43
1:C:40:VAL:HG22	1:C:44:SER:OG	2.19	0.43
1:C:58:VAL:CG1	1:C:63:PHE:HB2	2.46	0.43
2:A:151:TRP:CE3	2:A:152:THR:N	2.87	0.43
2:A:262:ILE:HG13	2:A:1617:ILE:HD13	2.00	0.43
2:A:338:ASP:OD2	2:A:342:THR:OG1	2.29	0.43
2:A:346:THR:HG22	2:A:347:PHE:N	2.34	0.43
2:A:401:VAL:HG11	2:A:960:LEU:HD22	2.00	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
1:C:101:PHE:CZ	1:C:105:PRO:HD3	2.54	0.42
2:A:207:LEU:HD12	2:A:213:LEU:HG	2.00	0.42
2:A:795:LEU:HD13	2:A:803:TYR:CZ	2.54	0.42
2:A:1408:TRP:HZ3	2:A:1441:ILE:CD1	2.32	0.42
2:A:1412:MET:CE	2:A:1434:TYR:HD1	2.29	0.42
2:A:1430:SER:C	2:A:1432:TYR:N	2.76	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1487:LYS:HA	2:A:1487:LYS:HD3	1.58	0.42
3:B:101:LEU:O	3:B:102:GLN:CB	2.65	0.42
3:B:178:MET:HG2	3:B:178:MET:H	1.63	0.42
1:C:30:MET:CG	1:C:137:ARG:C	2.86	0.42
1:C:34:VAL:HG23	1:C:35:PRO:O	2.18	0.42
1:C:65:LEU:C	1:C:65:LEU:CD2	2.86	0.42
2:A:1467:LEU:CD1	2:A:1472:ILE:CG2	2.90	0.42
3:B:67:PHE:N	3:B:67:PHE:HD1	2.17	0.42
1:C:30:MET:CG	1:C:138:GLY:HA2	2.37	0.42
1:C:59:ASN:HB3	1:C:62:GLN:CG	2.49	0.42
2:A:1286:ILE:HD12	2:A:1287:LYS:N	2.34	0.42
2:A:1420:ASN:CB	2:A:1423:LYS:HG3	2.50	0.42
2:A:1450:ASN:C	2:A:1450:ASN:ND2	2.73	0.42
2:A:1460:PHE:CD2	2:A:1756:ILE:HG13	2.53	0.42
2:A:845:LEU:HG	2:A:845:LEU:H	1.58	0.42
2:A:1522:MET:HE3	2:A:1522:MET:HA	2.02	0.42
2:A:333:ILE:CG2	2:A:334:GLY:N	2.83	0.42
2:A:911:ASN:O	2:A:911:ASN:ND2	2.40	0.42
2:A:1369:GLU:HG2	4:E:1:NAG:H62	2.00	0.42
3:B:67:PHE:CE2	3:B:120:GLU:CG	2.94	0.42
2:A:274:LYS:C	2:A:315:CYS:SG	3.02	0.42
2:A:854:MET:HE2	2:A:854:MET:HB2	1.63	0.42
2:A:1764:SER:HA	2:A:1767:THR:CG2	2.49	0.42
2:A:301:LYS:HZ1	3:B:131:ASN:CG	2.24	0.42
2:A:370:THR:O	2:A:374:ALA:HB3	2.19	0.42
2:A:406:LYS:HB2	2:A:406:LYS:HE2	1.78	0.42
2:A:1317:ALA:HA	2:A:1459:ASN:OD1	2.19	0.42
2:A:1373:LEU:O	2:A:1377:SER:N	2.52	0.42
3:B:71:LEU:HD22	3:B:106:ILE:HD11	2.00	0.42
2:A:380:ILE:O	2:A:384:VAL:HG12	2.19	0.42
2:A:1509:PHE:CA	2:A:1568:SER:OG	2.68	0.42
3:B:112:THR:CG2	3:B:113:TYR:H	2.33	0.42
1:C:47:ARG:C	1:C:49:PRO:HD3	2.43	0.42
2:A:128:PHE:HZ	2:A:166:GLU:HA	1.85	0.42
2:A:1325:LEU:HD13	2:A:1325:LEU:O	2.20	0.42
2:A:254:PHE:O	2:A:258:VAL:HG23	2.20	0.42
2:A:1340:VAL:O	2:A:1344:ALA:CB	2.68	0.42
2:A:1496:PRO:O	2:A:1497:ILE:CB	2.67	0.42
1:C:52:PHE:CB	1:C:129:ILE:CD1	2.82	0.41
2:A:842:VAL:O	2:A:845:LEU:CD1	2.67	0.41
2:A:1358:ARG:CZ	2:A:1417:ASP:OD2	2.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1539:GLN:O	2:A:1540:SER:CB	2.68	0.41
3:B:26:SER:OG	3:B:142:ILE:CG2	2.68	0.41
2:A:198:PHE:CE2	2:A:216:PHE:CD2	3.08	0.41
2:A:396:LEU:HD23	2:A:396:LEU:HA	1.76	0.41
2:A:739:PHE:O	2:A:742:MET:SD	2.78	0.41
2:A:748:LEU:C	2:A:748:LEU:CD1	2.86	0.41
2:A:803:TYR:HD2	2:A:804:PHE:CE1	2.39	0.41
2:A:1555:ILE:CD1	2:A:1593:MET:HE3	2.50	0.41
2:A:1722:PRO:CB	3:B:103:ASP:HB2	2.51	0.41
2:A:395:ASN:CG	2:A:1755:TYR:CD1	2.97	0.41
2:A:1295:LEU:HD13	2:A:1295:LEU:HA	1.89	0.41
2:A:1485:MET:CG	2:A:1639:MET:HE1	2.47	0.41
2:A:1500:PRO:HG2	2:A:1505:GLN:HB3	2.01	0.41
2:A:1614:LEU:HD12	2:A:1614:LEU:HA	1.87	0.41
3:B:32:TYR:CE2	3:B:113:TYR:HE1	2.18	0.41
3:B:59:PHE:CZ	3:B:61:GLN:HA	2.56	0.41
2:A:301:LYS:NZ	3:B:131:ASN:OD1	2.39	0.41
2:A:801:TYR:HD1	2:A:801:TYR:HA	1.76	0.41
2:A:1408:TRP:CZ3	2:A:1441:ILE:HD11	2.55	0.41
2:A:1566:LEU:HA	2:A:1566:LEU:HD12	1.75	0.41
2:A:1600:GLU:O	2:A:1603:PHE:CD1	2.74	0.41
2:A:1668:TYR:O	2:A:1729:ASP:HB2	2.19	0.41
2:A:1673:ASP:O	2:A:1702:GLY:O	2.39	0.41
3:B:162:MET:O	3:B:162:MET:SD	2.79	0.41
2:A:139:ASN:C	2:A:139:ASN:ND2	2.73	0.41
2:A:1547:LEU:HD23	2:A:1547:LEU:HA	1.85	0.41
2:A:1668:TYR:CE2	2:A:1726:VAL:HG21	2.56	0.41
3:B:59:PHE:CD2	3:B:119:TYR:CE1	3.08	0.41
1:C:52:PHE:HB3	1:C:129:ILE:HD13	1.98	0.41
2:A:147:ASN:ND2	2:A:147:ASN:O	2.53	0.41
2:A:219:LEU:HA	2:A:222:LEU:HD12	2.02	0.41
2:A:1594:PHE:HD1	2:A:1594:PHE:HA	1.77	0.41
2:A:1707:ILE:CG2	2:A:1736:GLY:HA3	2.51	0.41
3:B:32:TYR:CD1	3:B:33:GLY:N	2.88	0.41
2:A:175:GLY:CA	2:A:180:GLU:HA	2.50	0.41
2:A:286:LEU:C	2:A:286:LEU:CD2	2.94	0.41
2:A:1218:ARG:HD2	3:B:22:VAL:HG13	2.03	0.41
2:A:1543:MET:O	2:A:1543:MET:SD	2.79	0.41
2:A:1767:THR:HG23	2:A:1768:GLU:N	2.35	0.41
3:B:23:GLU:OE1	3:B:140:LYS:NZ	2.33	0.41
3:B:179:ILE:HD13	3:B:179:ILE:HA	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:VAL:HG12	1:C:50:CYS:SG	2.61	0.41
2:A:210:VAL:HG22	2:A:214:ARG:HG2	2.03	0.41
2:A:911:ASN:C	2:A:911:ASN:ND2	2.79	0.41
2:A:1456:ILE:HG21	2:A:1752:VAL:HG11	2.02	0.41
2:A:1508:ILE:CG2	2:A:1564:LEU:HD11	2.50	0.41
2:A:1663:MET:HE2	2:A:1663:MET:HB3	1.87	0.41
3:B:103:ASP:C	3:B:104:LEU:HD22	2.45	0.41
3:B:121:CYS:O	3:B:121:CYS:SG	2.79	0.41
2:A:174:ARG:CD	2:A:182:THR:HG21	2.16	0.41
2:A:180:GLU:HB2	2:A:183:PHE:HB3	2.02	0.41
2:A:365:ASN:HD22	2:A:365:ASN:HA	1.67	0.41
2:A:395:ASN:OD1	2:A:1755:TYR:HA	2.20	0.41
2:A:792:VAL:CG1	2:A:793:LEU:N	2.83	0.41
2:A:1306:GLY:HA2	2:A:1475:THR:CG2	2.50	0.41
2:A:1460:PHE:HD1	2:A:1460:PHE:HA	1.78	0.41
2:A:1553:VAL:HG12	2:A:1557:LEU:HD22	2.02	0.41
2:A:1583:PHE:CD1	2:A:1583:PHE:C	2.99	0.41
2:A:1596:ALA:CB	2:A:1609:PHE:CE2	2.85	0.41
2:A:1677:ASP:OD1	2:A:1677:ASP:N	2.53	0.41
3:B:44:LYS:NZ	3:B:100:ASP:OD2	2.54	0.41
2:A:403:MET:O	2:A:403:MET:SD	2.79	0.41
2:A:758:THR:CG2	2:A:759:LEU:N	2.84	0.41
2:A:1634:LEU:HD12	2:A:1634:LEU:HA	1.86	0.41
2:A:1639:MET:CE	2:A:1639:MET:CA	2.85	0.41
3:B:46:ARG:NH2	3:B:48:GLU:OE1	2.53	0.41
1:C:59:ASN:CB	1:C:62:GLN:CB	2.86	0.40
2:A:272:LYS:O	2:A:274:LYS:HG3	2.21	0.40
2:A:851:THR:O	2:A:854:MET:HB3	2.21	0.40
2:A:909:HIS:CD2	2:A:909:HIS:C	2.98	0.40
2:A:1326:LEU:HD22	2:A:1326:LEU:HA	1.81	0.40
2:A:1647:ILE:HG23	2:A:1750:VAL:HG13	2.02	0.40
2:A:146:ASN:O	2:A:147:ASN:CB	2.69	0.40
2:A:176:PHE:CD2	2:A:178:VAL:CG2	3.05	0.40
2:A:798:MET:O	2:A:799:ASP:CB	2.70	0.40
2:A:952:MET:O	2:A:956:ASN:HB2	2.21	0.40
2:A:1268:VAL:HG13	2:A:1289:LEU:HD13	2.02	0.40
3:B:32:TYR:HE2	3:B:113:TYR:CD1	2.30	0.40
2:A:164:THR:O	2:A:168:LEU:HB3	2.22	0.40
2:A:1238:ILE:CD1	2:A:1270:LEU:HD21	2.40	0.40
2:A:1580:ILE:O	2:A:1584:VAL:HG23	2.21	0.40
3:B:79:GLN:HE21	3:B:79:GLN:HB2	1.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:971:PHE:CD1	2:A:972:SER:HB2	2.56	0.40
2:A:1241:MET:O	2:A:1244:LYS:HB2	2.22	0.40
2:A:1408:TRP:HZ3	2:A:1441:ILE:HD11	1.87	0.40
2:A:1412:MET:O	2:A:1416:VAL:HG13	2.22	0.40
2:A:1511:LEU:HD21	2:A:1517:PHE:CD2	2.57	0.40
2:A:1545:GLU:OE1	2:A:1545:GLU:CA	2.70	0.40
2:A:1666:PHE:O	2:A:1669:VAL:HG22	2.21	0.40
2:A:1737:ILE:O	2:A:1741:VAL:HG23	2.21	0.40
2:A:251:LEU:HD13	2:A:1630:ILE:CG2	2.46	0.40
2:A:338:ASP:O	2:A:339:TYR:CB	2.70	0.40
2:A:742:MET:HB2	2:A:746:VAL:CG2	2.51	0.40
2:A:1360:PRO:O	2:A:1361:ALA:CB	2.69	0.40
2:A:1457:ILE:CD1	2:A:1458:ASP:N	2.73	0.40
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%)	4	27
2	A	1132/2031 (56%)	1096 (97%)	20 (2%)	16 (1%)	9	39
3	B	171/218 (78%)	167 (98%)	4 (2%)	0	100	100
All	All	1421/2464 (58%)	1373 (97%)	29 (2%)	19 (1%)	12	40

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	147	ASN
2	A	896	VAL
2	A	1431	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	841	ARG
2	A	844	LYS
2	A	1213	ASP
2	A	1294	ALA
2	A	1540	SER
1	C	56	TYR
1	C	76	SER
2	A	305	TYR
2	A	903	CYS
2	A	1386	LYS
2	A	1497	ILE
2	A	1605	SER
1	C	147	LEU
2	A	1498	PRO
2	A	1604	VAL
2	A	767	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	113/193 (58%)	97 (86%)	16 (14%)	3	17
2	A	1018/1809 (56%)	738 (72%)	280 (28%)	0	2
3	B	157/190 (83%)	103 (66%)	54 (34%)	0	0
All	All	1288/2192 (59%)	938 (73%)	350 (27%)	2	2

All (350) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	30	MET
1	C	34	VAL
1	C	48	LEU
1	C	51	THR
1	C	52	PHE
1	C	59	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	61	LYS
1	C	65	LEU
1	C	74	ASN
1	C	107	LYS
1	C	129	ILE
1	C	130	MET
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
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	143	MET
2	A	145	MET
2	A	146	ASN
2	A	147	ASN
2	A	153	LYS
2	A	166	GLU
2	A	167	SER
2	A	168	LEU
2	A	171	ILE
2	A	181	PHE
2	A	184	LEU
2	A	191	LEU
2	A	192	ASP
2	A	196	ILE
2	A	206	ASN
2	A	207	LEU
2	A	209	ASN
2	A	214	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	215	THR
2	A	217	ARG
2	A	220	ARG
2	A	227	VAL
2	A	231	LEU
2	A	235	VAL
2	A	238	LEU
2	A	243	LYS
2	A	247	ASP
2	A	249	MET
2	A	255	CYS
2	A	271	LEU
2	A	280	LEU
2	A	285	THR
2	A	286	LEU
2	A	291	ASN
2	A	293	LEU
2	A	298	ASP
2	A	300	ARG
2	A	310	LYS
2	A	311	ASP
2	A	313	LEU
2	A	314	LEU
2	A	318	SER
2	A	329	THR
2	A	348	SER
2	A	349	TRP
2	A	354	LEU
2	A	356	ARG
2	A	358	MET
2	A	364	GLU
2	A	365	ASN
2	A	366	LEU
2	A	370	THR
2	A	371	LEU
2	A	379	MET
2	A	387	PHE
2	A	403	MET
2	A	406	LYS
2	A	408	GLN
2	A	410	GLN
2	A	412	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	414	GLU
2	A	415	GLU
2	A	726	CYS
2	A	727	SER
2	A	729	TYR
2	A	732	LYS
2	A	733	PHE
2	A	734	LYS
2	A	736	CYS
2	A	748	LEU
2	A	750	ILE
2	A	751	THR
2	A	755	VAL
2	A	759	LEU
2	A	763	MET
2	A	764	GLU
2	A	765	HIS
2	A	766	HIS
2	A	768	MET
2	A	769	THR
2	A	771	GLU
2	A	773	LYS
2	A	774	ASN
2	A	776	LEU
2	A	780	ASN
2	A	781	LEU
2	A	790	GLU
2	A	791	MET
2	A	794	LYS
2	A	795	LEU
2	A	796	ILE
2	A	798	MET
2	A	801	TYR
2	A	808	TRP
2	A	815	ILE
2	A	818	LEU
2	A	820	LEU
2	A	821	VAL
2	A	825	LEU
2	A	831	LEU
2	A	834	LEU
2	A	835	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	837	PHE
2	A	838	ARG
2	A	839	LEU
2	A	840	LEU
2	A	841	ARG
2	A	845	LEU
2	A	848	SER
2	A	854	MET
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	896	VAL
2	A	898	LYS
2	A	901	ASP
2	A	905	LEU
2	A	910	MET
2	A	916	SER
2	A	918	LEU
2	A	924	LEU
2	A	929	ILE
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	1204	LEU
2	A	1206	SER
2	A	1209	LEU
2	A	1212	GLU
2	A	1214	ILE
2	A	1218	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	1219	LYS
2	A	1223	LYS
2	A	1225	ILE
2	A	1226	LEU
2	A	1232	ILE
2	A	1246	ILE
2	A	1251	LYS
2	A	1264	LEU
2	A	1265	ILE
2	A	1270	LEU
2	A	1274	VAL
2	A	1277	THR
2	A	1278	LEU
2	A	1283	LEU
2	A	1286	ILE
2	A	1287	LYS
2	A	1289	LEU
2	A	1290	ARG
2	A	1293	ARG
2	A	1295	LEU
2	A	1296	ARG
2	A	1299	ARG
2	A	1305	GLU
2	A	1307	MET
2	A	1309	VAL
2	A	1323	ASN
2	A	1325	LEU
2	A	1326	LEU
2	A	1342	LEU
2	A	1350	CYS
2	A	1353	THR
2	A	1354	THR
2	A	1358	ARG
2	A	1366	ASN
2	A	1369	GLU
2	A	1385	LEU
2	A	1399	LEU
2	A	1409	THR
2	A	1416	VAL
2	A	1419	VAL
2	A	1422	ASP
2	A	1423	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	1424	GLN
2	A	1426	LYS
2	A	1449	LEU
2	A	1450	ASN
2	A	1452	PHE
2	A	1462	GLN
2	A	1464	LYS
2	A	1465	LYS
2	A	1467	LEU
2	A	1472	ILE
2	A	1474	MET
2	A	1478	GLN
2	A	1479	LYS
2	A	1480	LYS
2	A	1486	LYS
2	A	1487	LYS
2	A	1488	LEU
2	A	1491	LYS
2	A	1495	LYS
2	A	1497	ILE
2	A	1503	LYS
2	A	1504	ILE
2	A	1511	LEU
2	A	1515	GLN
2	A	1517	PHE
2	A	1519	ILE
2	A	1520	SER
2	A	1524	LEU
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	1541	GLN
2	A	1543	MET
2	A	1545	GLU
2	A	1557	LEU
2	A	1561	GLU
2	A	1562	CYS
2	A	1565	LYS
2	A	1566	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	1570	ARG
2	A	1571	HIS
2	A	1573	TYR
2	A	1593	MET
2	A	1594	PHE
2	A	1598	LEU
2	A	1601	THR
2	A	1602	TYR
2	A	1605	SER
2	A	1608	LEU
2	A	1614	LEU
2	A	1616	ARG
2	A	1619	ARG
2	A	1620	ILE
2	A	1621	LEU
2	A	1628	LYS
2	A	1634	LEU
2	A	1637	LEU
2	A	1644	LEU
2	A	1649	LEU
2	A	1653	LEU
2	A	1670	LYS
2	A	1671	LYS
2	A	1672	GLU
2	A	1673	ASP
2	A	1683	THR
2	A	1687	SER
2	A	1691	LEU
2	A	1704	LEU
2	A	1707	ILE
2	A	1711	LYS
2	A	1719	LYS
2	A	1725	SER
2	A	1726	VAL
2	A	1727	GLU
2	A	1749	LEU
2	A	1753	ASN
2	A	1754	MET
3	B	27	GLU
3	B	28	THR
3	B	29	GLU
3	B	34	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	37	LYS
3	B	39	LEU
3	B	45	ARG
3	B	46	ARG
3	B	47	SER
3	B	48	GLU
3	B	50	ASN
3	B	65	GLU
3	B	66	GLU
3	B	67	PHE
3	B	69	LYS
3	B	76	GLU
3	B	78	LEU
3	B	79	GLN
3	B	80	LEU
3	B	82	GLU
3	B	84	GLU
3	B	85	ARG
3	B	90	VAL
3	B	93	ASN
3	B	95	SER
3	B	96	ARG
3	B	99	LYS
3	B	101	LEU
3	B	102	GLN
3	B	104	LEU
3	B	106	ILE
3	B	109	THR
3	B	121	CYS
3	B	125	ARG
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	149	LYS
3	B	152	ARG
3	B	159	SER
3	B	166	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	174	LEU
3	B	178	MET
3	B	180	TYR
3	B	181	CYS
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 (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	136	HIS
1	C	145	GLN
2	A	139	ASN
2	A	147	ASN
2	A	154	ASN
2	A	278	ASN
2	A	291	ASN
2	A	360	GLN
2	A	365	ASN
2	A	408	GLN
2	A	410	GLN
2	A	766	HIS
2	A	774	ASN
2	A	909	HIS
2	A	941	GLN
2	A	956	ASN
2	A	1180	ASN
2	A	1276	ASN
2	A	1378	GLN
2	A	1424	GLN
2	A	1450	ASN
2	A	1514	ASN
2	A	1528	ASN
2	A	1551	ASN
2	A	1571	HIS
2	A	1753	ASN
2	A	1762	ASN
3	B	50	ASN
3	B	79	GLN
3	B	102	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	115	HIS
3	B	134	HIS
3	B	143	HIS

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	0.44	0	17,19,21	0.92	0
4	NAG	D	2	4	14,14,15	0.42	0	17,19,21	1.32	3 (17%)
4	NAG	E	1	2,4	14,14,15	0.37	0	17,19,21	1.07	2 (11%)
4	NAG	E	2	4	14,14,15	0.40	0	17,19,21	1.12	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	2	4	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1	NAG	O5-C1-C2	-3.16	106.40	111.29
4	E	2	NAG	C1-O5-C5	-3.07	108.07	112.19
4	D	2	NAG	C2-N2-C7	-2.77	119.19	122.90
4	D	2	NAG	C1-O5-C5	2.72	115.83	112.19
4	E	1	NAG	O4-C4-C3	-2.15	105.31	110.38
4	D	2	NAG	C1-C2-N2	2.01	113.60	110.43

There are no chirality outliers.

All (15) torsion outliers are listed below:

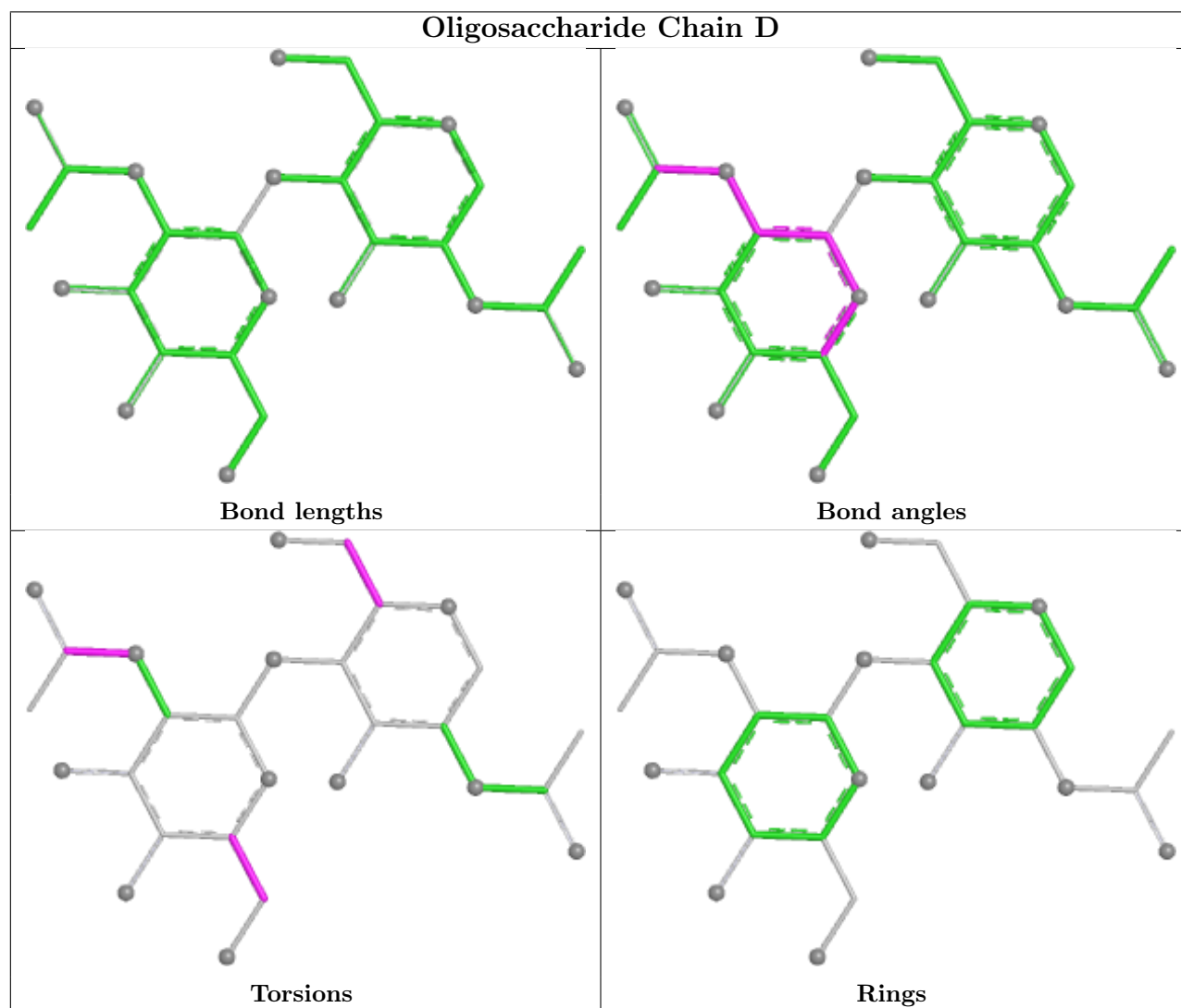
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C1-C2-N2-C7
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
4	D	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	E	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C3-C2-N2-C7
4	E	1	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	E	1	NAG	C3-C2-N2-C7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

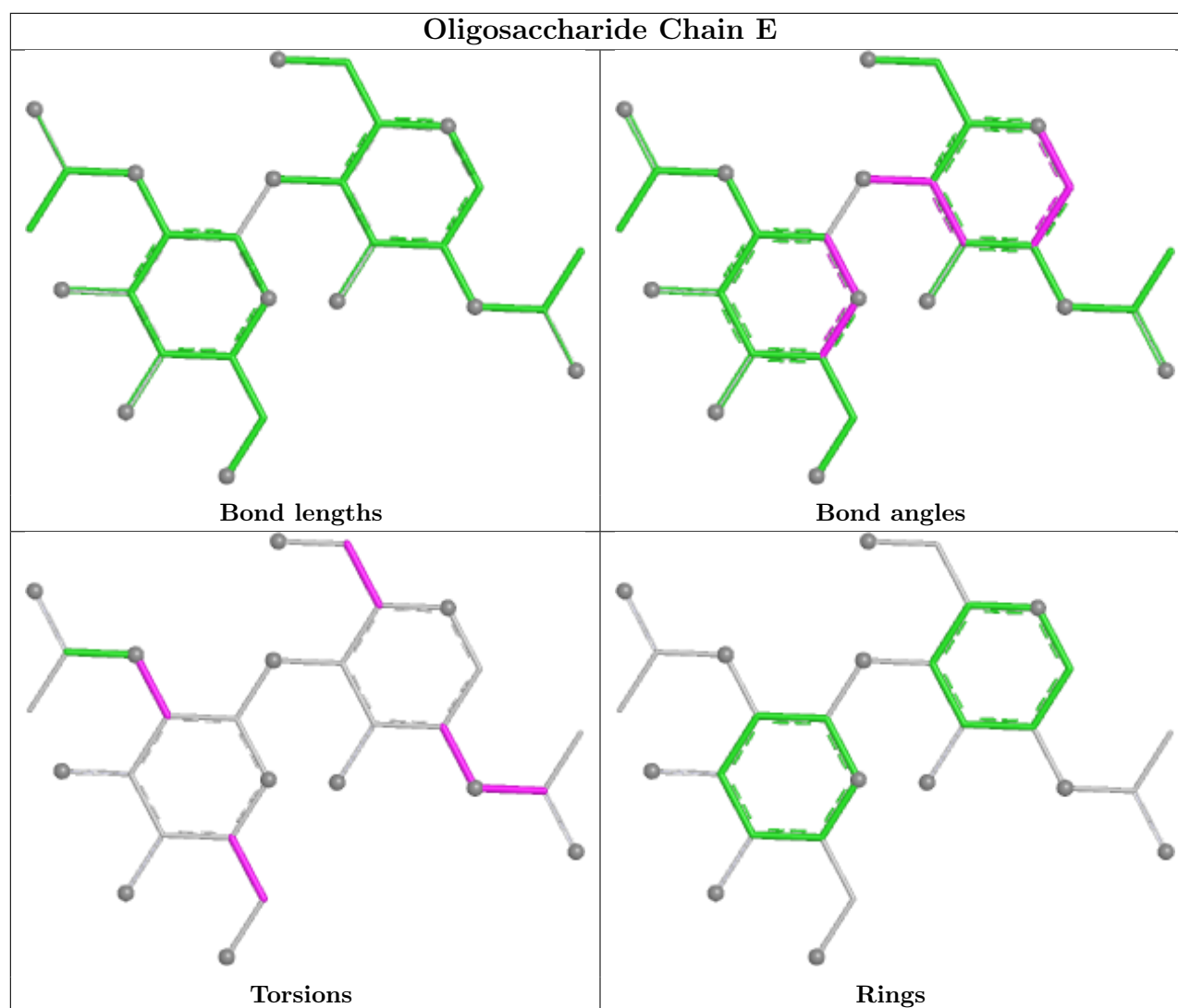
There are no ring outliers.

2 monomers are involved in 6 short contacts:

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





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	0.36	0	17,19,21	0.38	0
5	NAG	A	2005	2	14,14,15	2.85	1 (7%)	17,19,21	2.33	2 (11%)
5	NAG	B	304	3	14,14,15	0.39	0	17,19,21	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	9SL	A	2007	-	17,23,23	3.63	8 (47%)	14,37,37	3.00	7 (50%)
5	NAG	B	303	3	14,14,15	0.34	0	17,19,21	0.50	0
5	NAG	B	302	3	14,14,15	0.37	0	17,19,21	0.47	0
5	NAG	B	301	3	14,14,15	0.44	0	17,19,21	1.05	0
5	NAG	A	2006	2	14,14,15	0.37	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	A	2005	2	-	2/6/23/26	0/1/1/1
5	NAG	B	304	3	-	2/6/23/26	0/1/1/1
6	9SL	A	2007	-	-	4/5/53/53	0/3/3/3
5	NAG	B	303	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	301	3	-	5/6/23/26	0/1/1/1
5	NAG	A	2006	2	-	2/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2005	NAG	C1-C2	10.56	1.66	1.52
6	A	2007	9SL	C12-N13	8.73	1.49	1.35
6	A	2007	9SL	C07-N08	6.23	1.45	1.34
6	A	2007	9SL	C02-N21	6.10	1.44	1.33
6	A	2007	9SL	C12-N15	4.61	1.45	1.34
6	A	2007	9SL	C05-C14	4.10	1.60	1.52
6	A	2007	9SL	O03-C02	2.90	1.39	1.35
6	A	2007	9SL	O01-C02	-2.85	1.17	1.22
6	A	2007	9SL	C05-N06	-2.69	1.43	1.47

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2005	NAG	C1-O5-C5	-8.33	101.03	112.19
6	A	2007	9SL	O03-C02-N21	7.79	120.80	111.11
5	A	2005	NAG	O5-C1-C2	-4.68	104.05	111.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2007	9SL	O01-C02-N21	-4.45	118.55	125.58
6	A	2007	9SL	N09-C07-N06	-3.32	120.80	125.42
6	A	2007	9SL	N13-C12-N11	-3.07	107.65	115.62
6	A	2007	9SL	O03-C02-O01	-2.64	120.64	123.08
6	A	2007	9SL	O03-C04-C05	2.30	112.96	108.46
6	A	2007	9SL	C14-C05-N06	2.13	117.04	111.22

There are no chirality outliers.

All (21) torsion outliers are listed below:

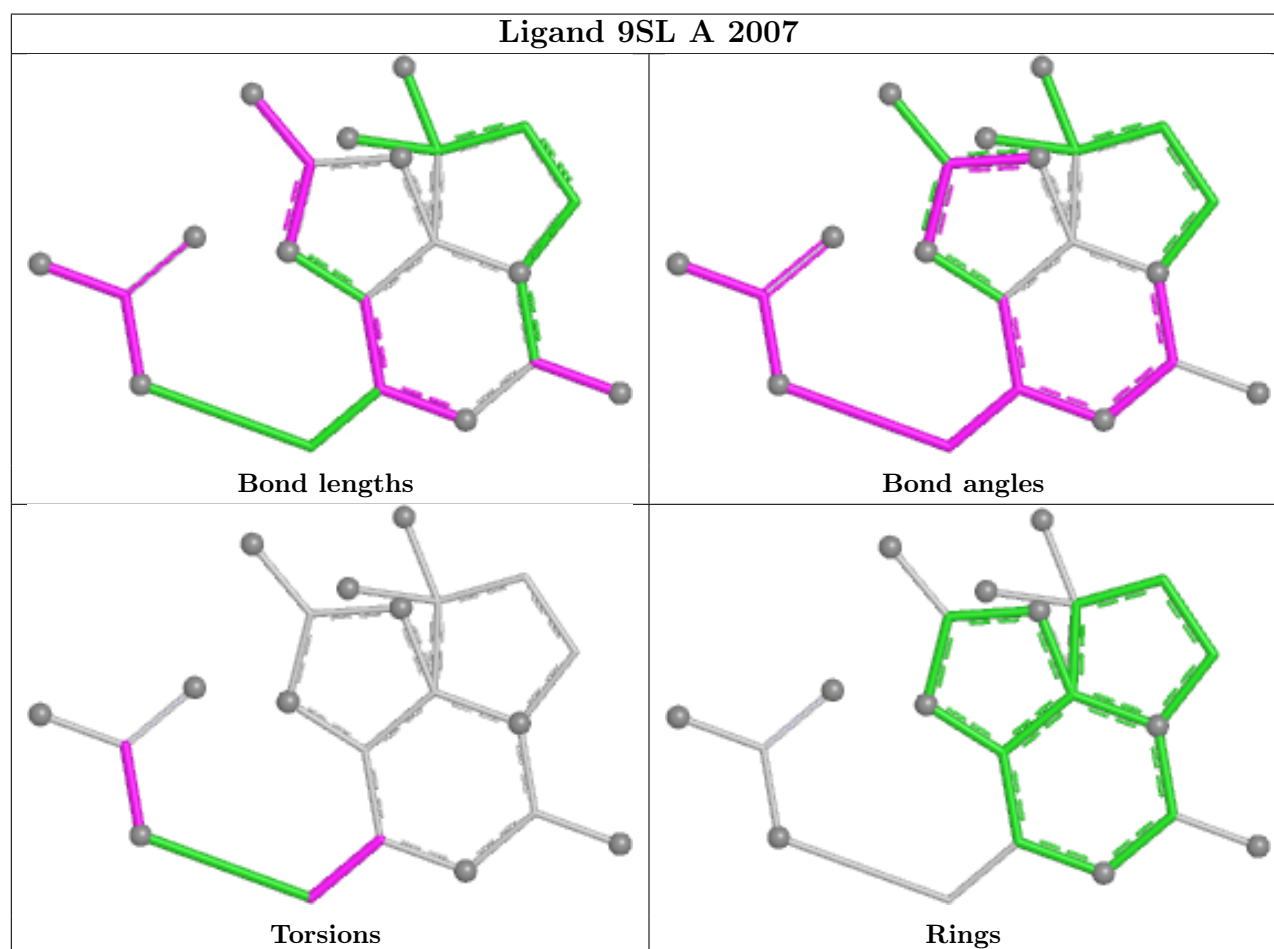
Mol	Chain	Res	Type	Atoms
5	B	301	NAG	C8-C7-N2-C2
5	B	301	NAG	O7-C7-N2-C2
6	A	2007	9SL	O01-C02-O03-C04
6	A	2007	9SL	N21-C02-O03-C04
6	A	2007	9SL	O03-C04-C05-N06
6	A	2007	9SL	O03-C04-C05-C14
5	C	301	NAG	O5-C5-C6-O6
5	A	2005	NAG	O5-C5-C6-O6
5	A	2006	NAG	O5-C5-C6-O6
5	B	303	NAG	O5-C5-C6-O6
5	B	304	NAG	O5-C5-C6-O6
5	B	301	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	304	NAG	C4-C5-C6-O6
5	B	303	NAG	C4-C5-C6-O6
5	B	301	NAG	C4-C5-C6-O6
5	B	302	NAG	C4-C5-C6-O6
5	B	301	NAG	C3-C2-N2-C7
5	B	302	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	301	NAG	5	0
5	A	2005	NAG	1	0
6	A	2007	9SL	2	0
5	A	2006	NAG	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 than 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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

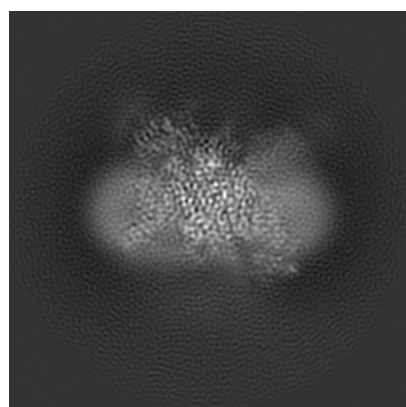
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9781. These allow visual inspection of the internal detail of the map and identification of artifacts.

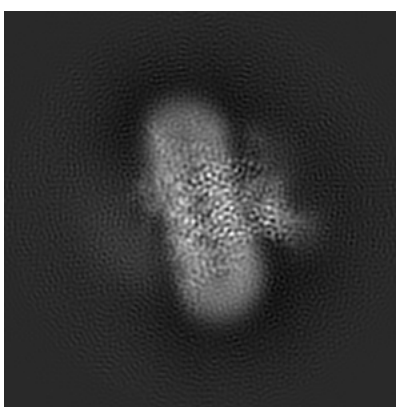
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

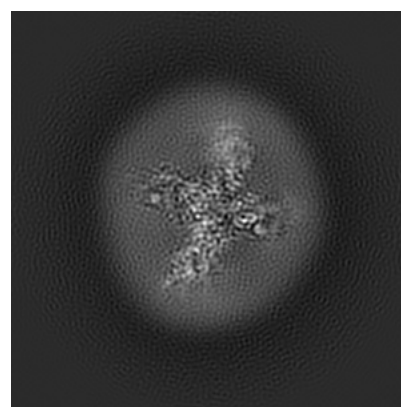
6.1.1 Primary map



X



Y

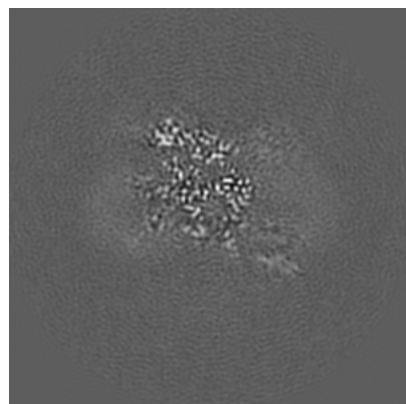


Z

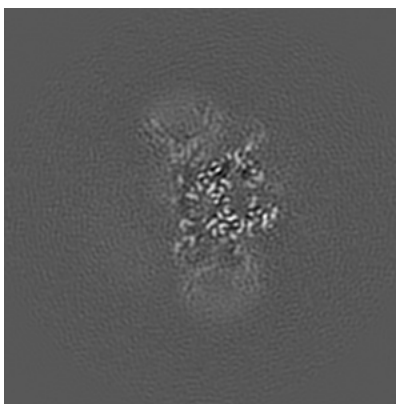
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

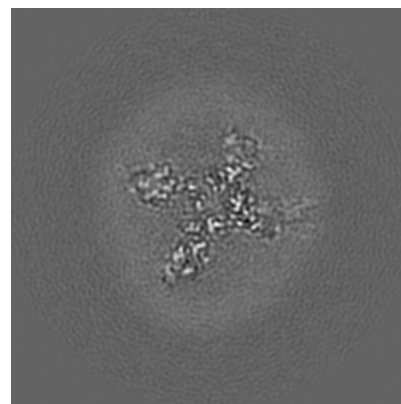
6.2.1 Primary map



X Index: 120



Y Index: 120

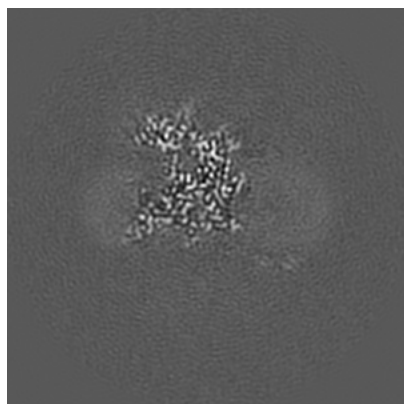


Z Index: 120

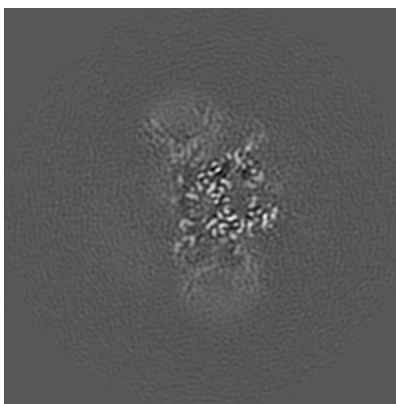
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

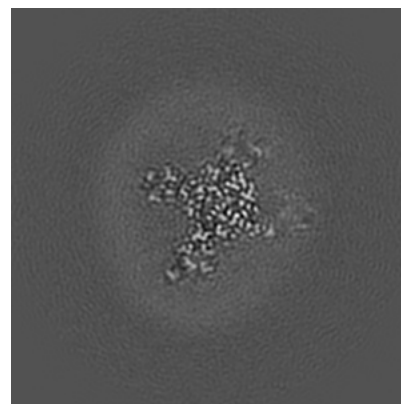
6.3.1 Primary map



X Index: 112



Y Index: 120

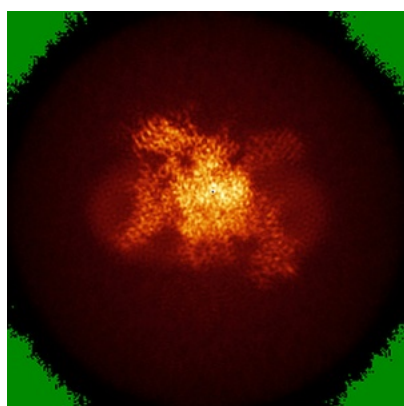


Z Index: 127

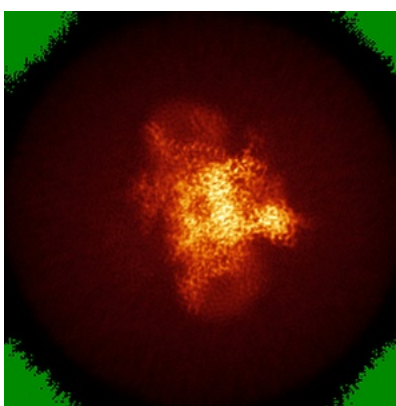
The images above show the largest variance slices of the map in three orthogonal directions.

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

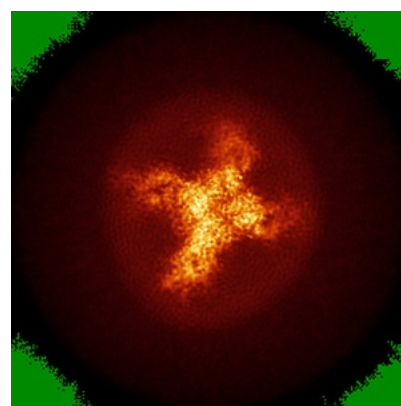
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

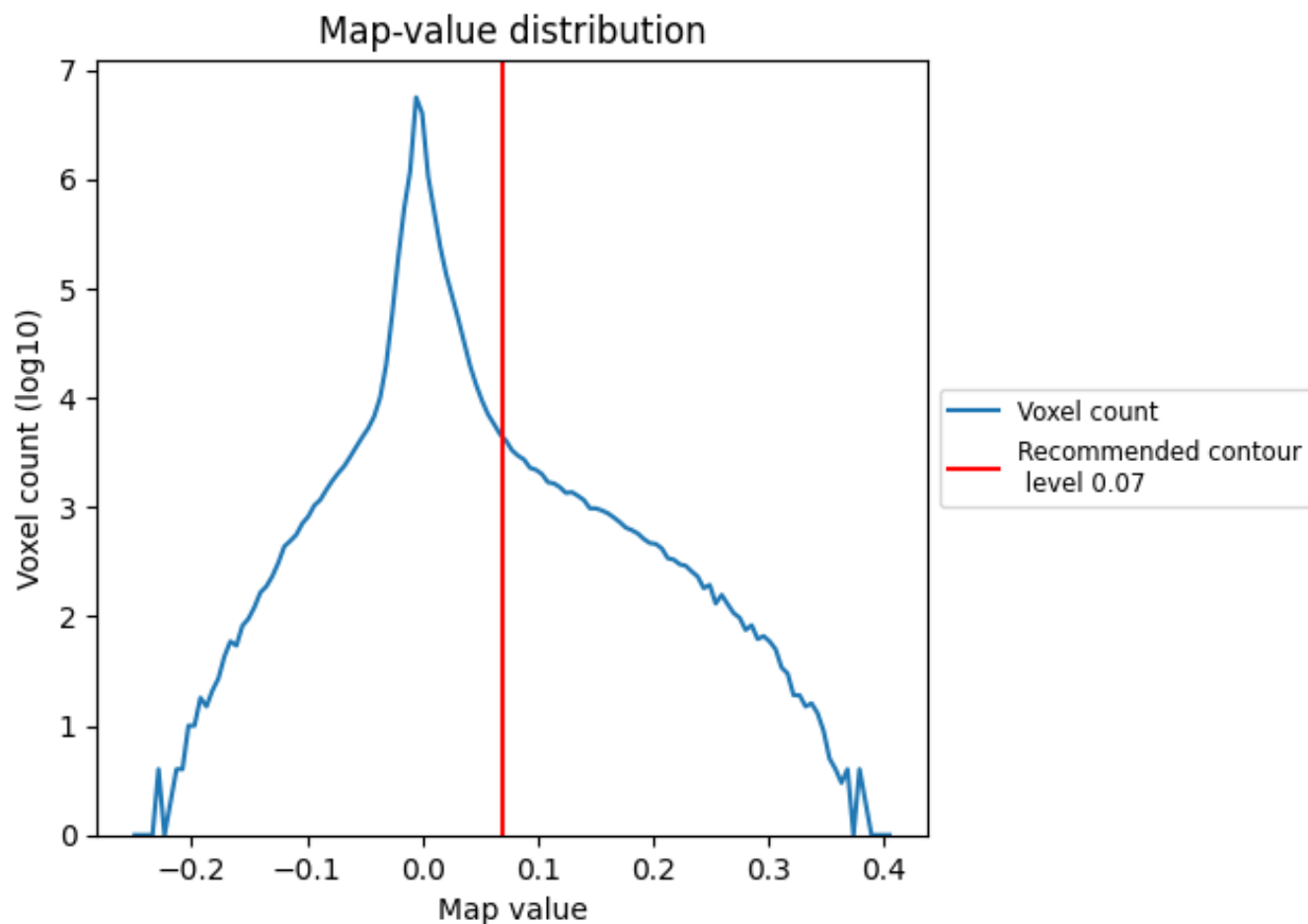
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

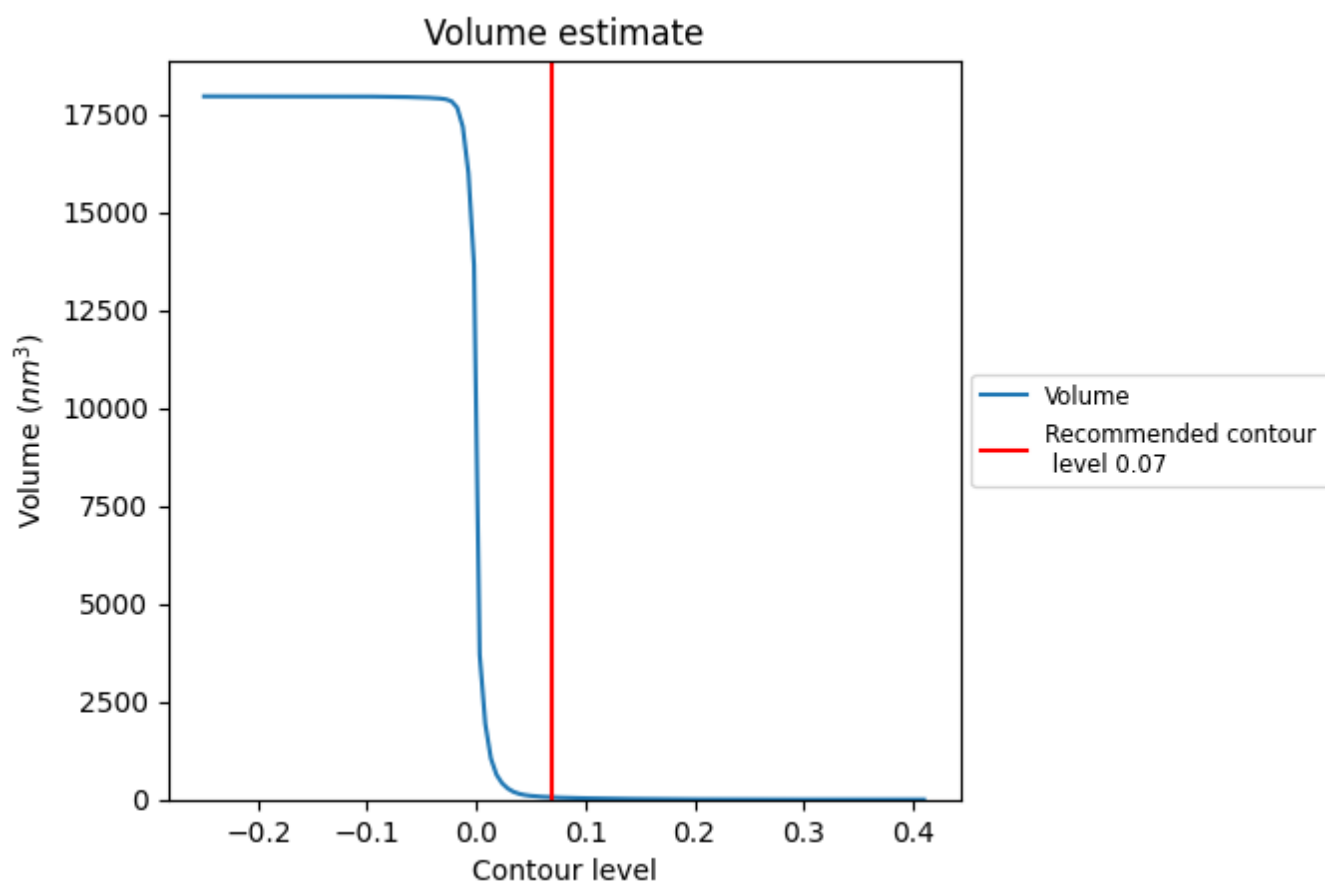
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

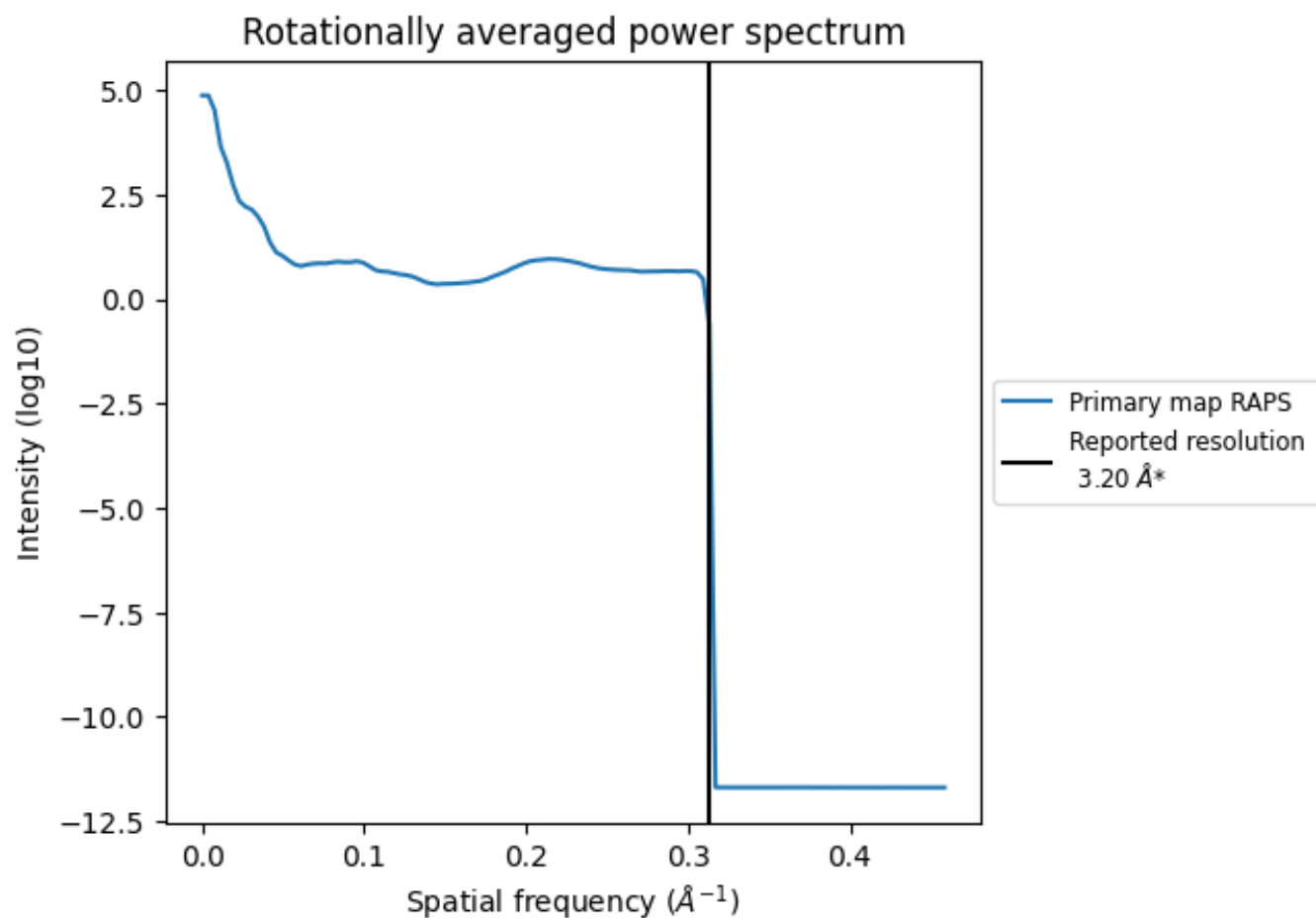
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 57 nm³; 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

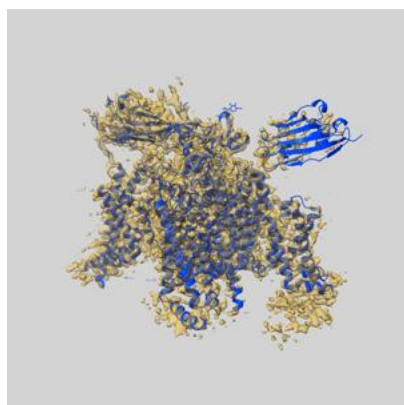
8 Fourier-Shell correlation

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

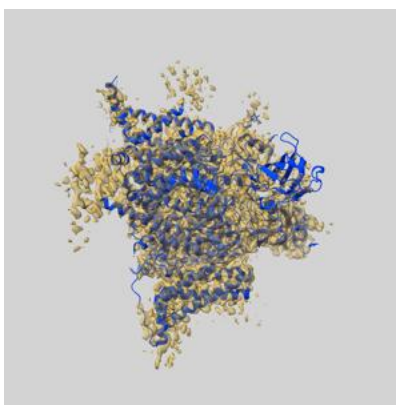
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9781 and PDB model 6J8G. Per-residue inclusion information can be found in section [3](#) on page [8](#).

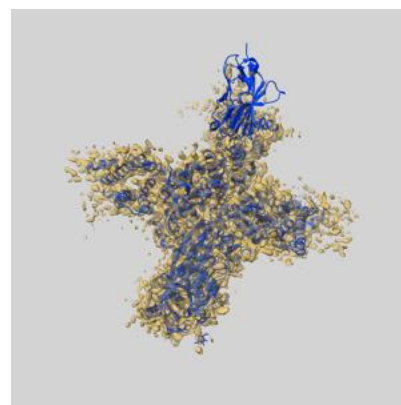
9.1 Map-model overlay [i](#)



X



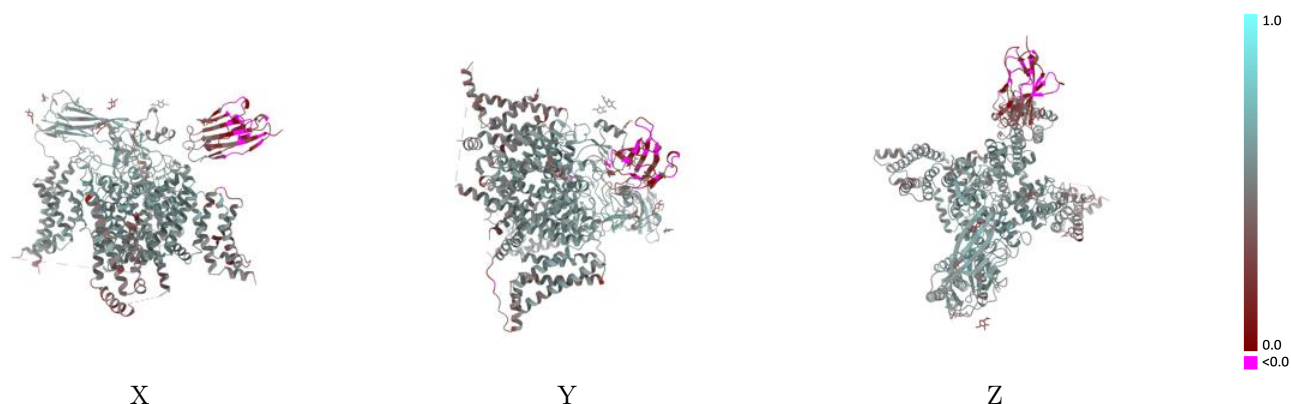
Y



Z

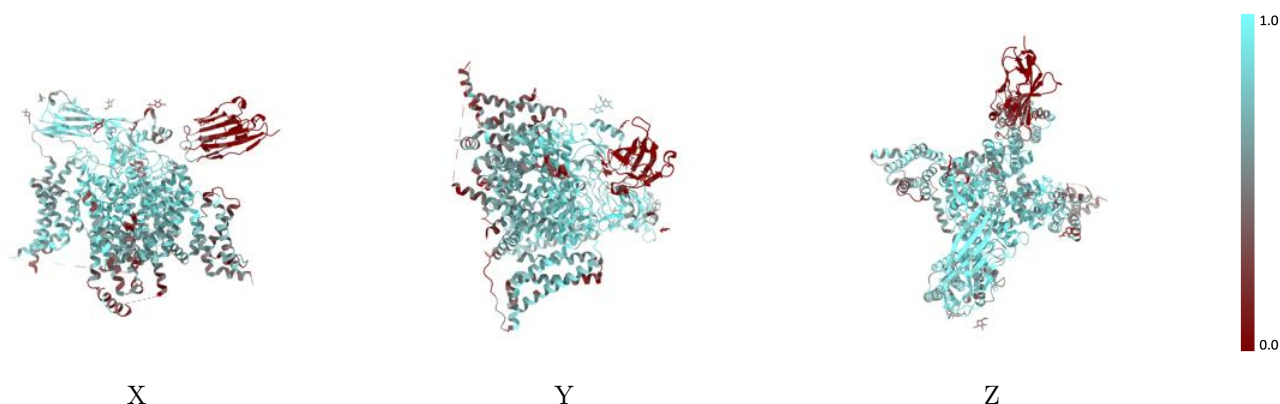
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



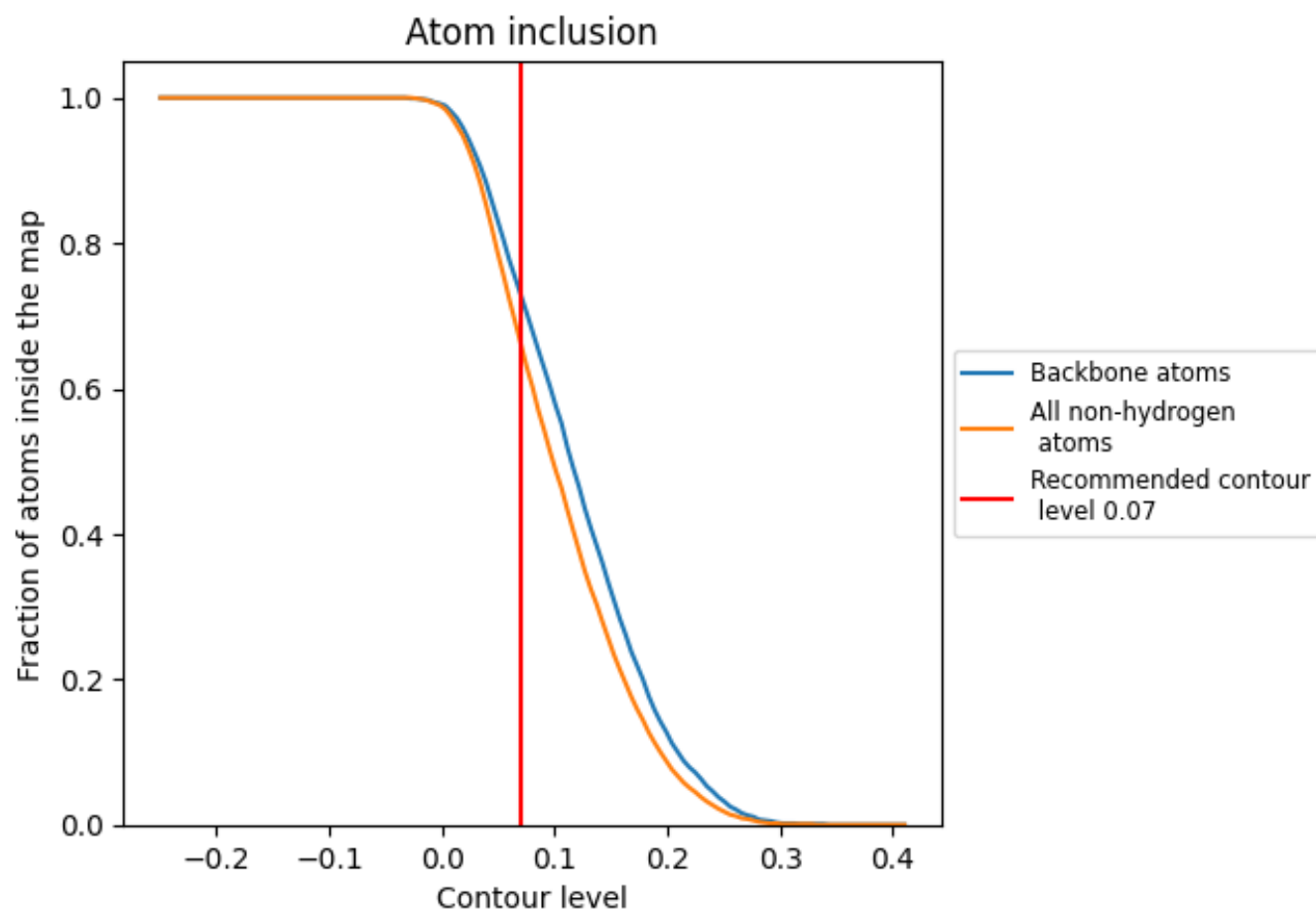
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 66% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6610	0.4950
A	0.7090	0.5250
B	0.7400	0.5180
C	0.1070	0.1800
D	0.3930	0.3450
E	0.6430	0.4580

