



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jul 24, 2017 – 02:00 AM EDT

PDB ID : 5A63
EMDB ID: : EMD-3061
Title : Cryo-EM structure of the human gamma-secretase complex at 3.4 angstrom resolution.
Authors : Bai, X.; Yan, C.; Yang, G.; Lu, P.; Ma, D.; Sun, L.; Zhou, R.; Scheres, S.H.W.; Shi, Y.
Deposited on : unknown
Resolution : 3.40 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

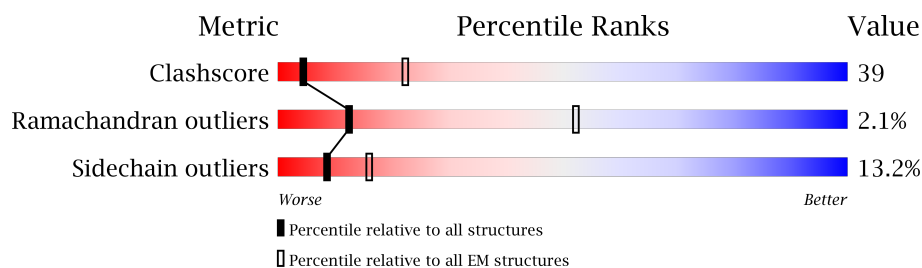
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	709	
2	B	467	
3	C	265	
4	D	101	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10003 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 NICASTRIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	665	Total	C	N	O	S	0	0
			5222	3312	888	1001	21		

- Molecule 2 is a protein called PRESENILIN-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	215	Total	C	N	O	S	0	0
			1702	1170	249	274	9		

- Molecule 3 is a protein called GAMMA-SECRETASE SUBUNIT APH-1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	243	Total	C	N	O	S	0	0
			1872	1254	299	315	4		

- Molecule 4 is a protein called GAMMA-SECRETASE SUBUNIT PEN-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	100	Total	C	N	O	S	0	0
			850	580	134	135	1		

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



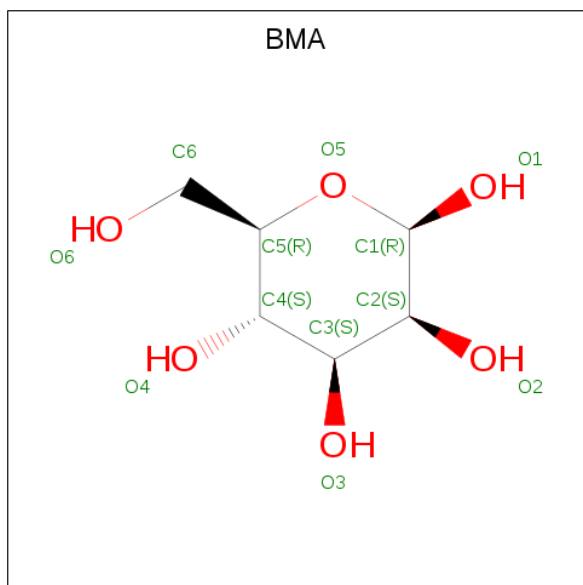
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			238	136	17	85	
5	A	1	Total	C	N	O	0
			238	136	17	85	
5	A	1	Total	C	N	O	0
			238	136	17	85	
5	A	1	Total	C	N	O	0
			238	136	17	85	
5	A	1	Total	C	N	O	0
			238	136	17	85	
5	A	1	Total	C	N	O	0
			238	136	17	85	
5	A	1	Total	C	N	O	0
			238	136	17	85	
5	A	1	Total	C	N	O	0
			238	136	17	85	
5	A	1	Total	C	N	O	0
			238	136	17	85	
5	A	1	Total	C	N	O	0
			238	136	17	85	
5	A	1	Total	C	N	O	0
			238	136	17	85	
5	A	1	Total	C	N	O	0
			238	136	17	85	

Continued on next page...

Continued from previous page...

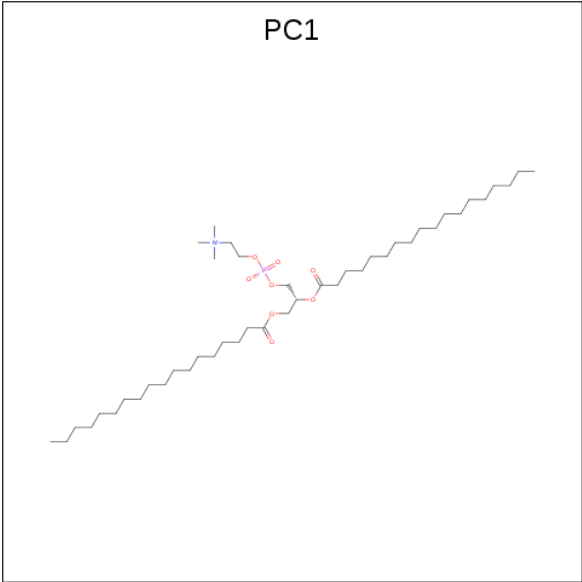
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			238	136	17	85	
5	A	1	Total	C	N	O	0
			238	136	17	85	
5	A	1	Total	C	N	O	0
			238	136	17	85	

- Molecule 6 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			33	18	15	
6	A	1	Total	C	O	0
			33	18	15	
6	A	1	Total	C	O	0
			33	18	15	

- Molecule 7 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).

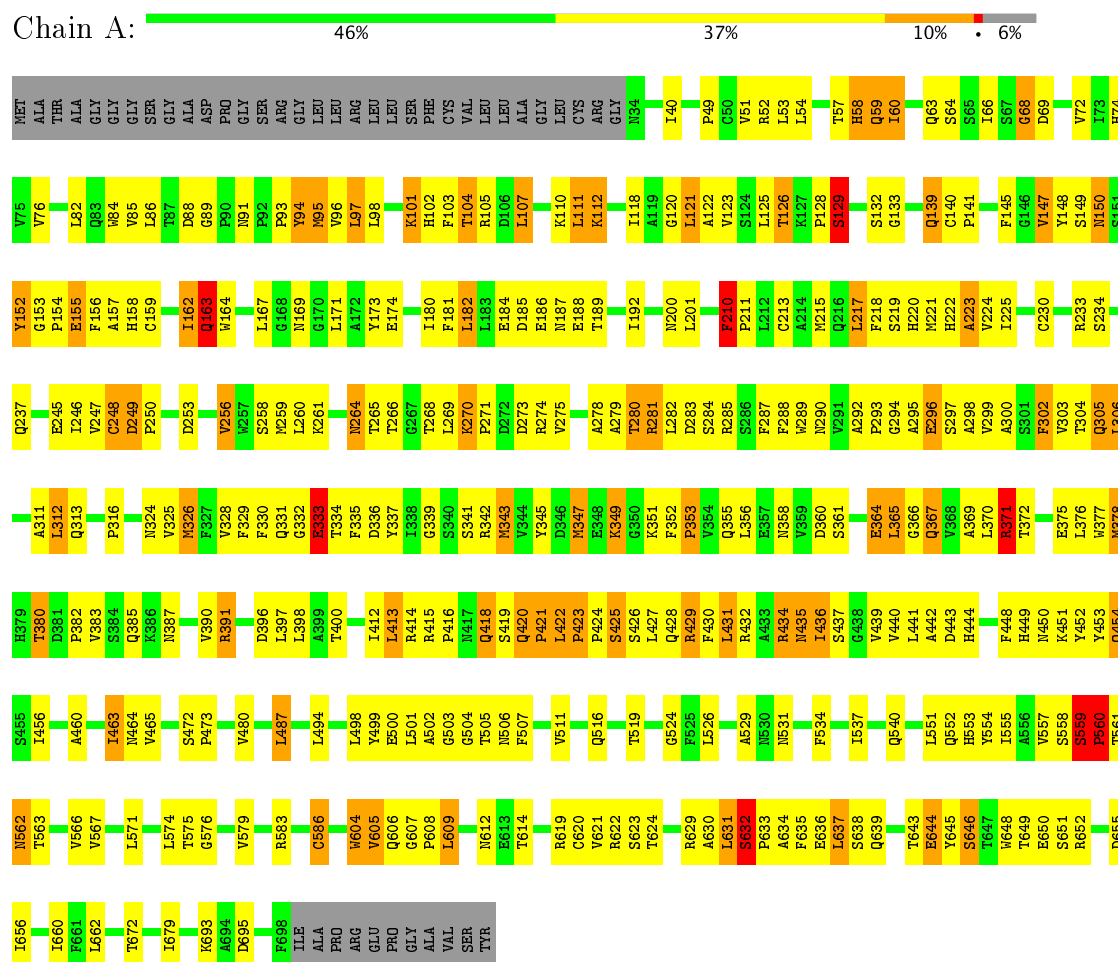


Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total	C	N	O	P	0
			43	33	1	8	1	
7	C	1	Total	C	N	O	P	0
			43	33	1	8	1	

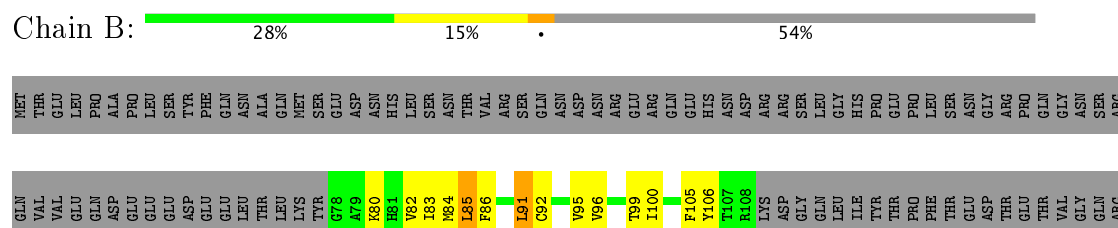
3 Residue-property plots

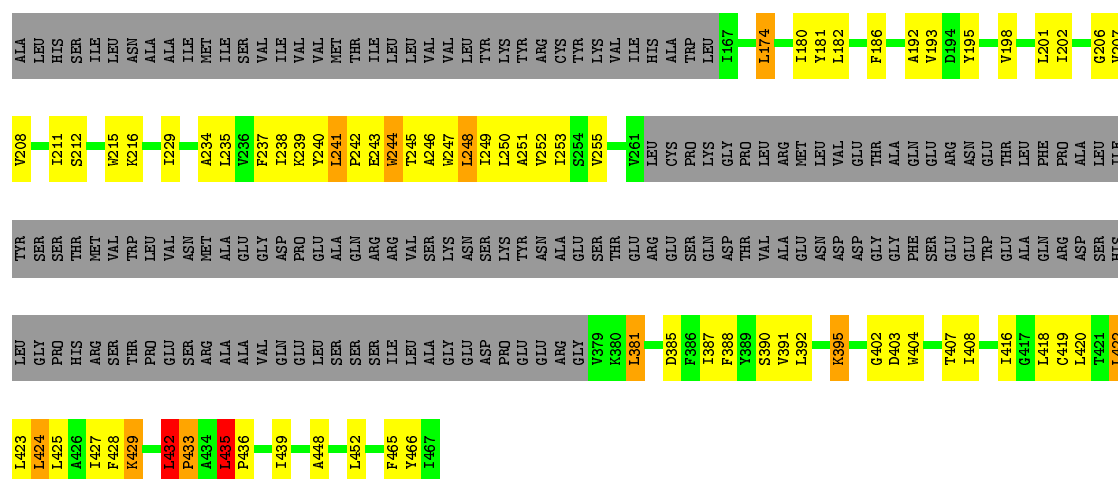
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

• Molecule 1: NICASTRIN



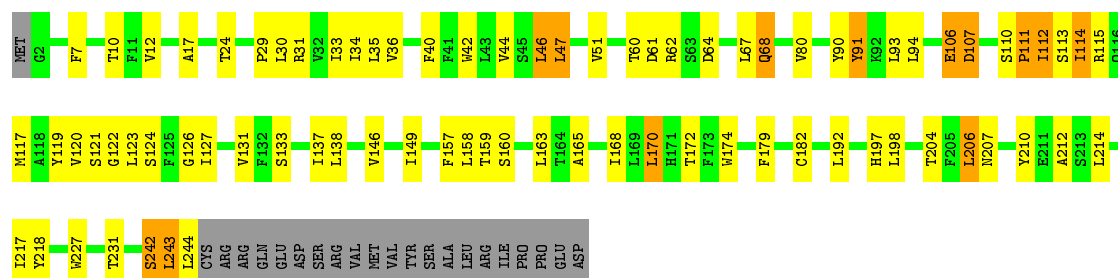
• Molecule 2: PRESENILIN-1





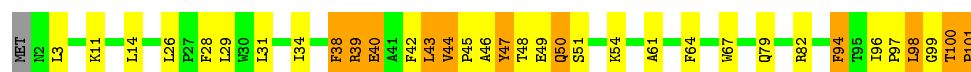
• Molecule 3: GAMMA-SECRETASE SUBUNIT APH-1A

Chain C: 62% 25% 5% 8%



• Molecule 4: GAMMA-SECRETASE SUBUNIT PEN-2

Chain D: 65% 23% 11%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	159549	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	35714	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, PC1

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 >2	RMSZ	# Z >2
1	A	0.54	3/5345 (0.1%)	0.75	8/7284 (0.1%)
2	B	0.46	1/1748 (0.1%)	0.76	1/2385 (0.0%)
3	C	0.48	1/1924 (0.1%)	0.78	1/2624 (0.0%)
4	D	0.53	1/883 (0.1%)	0.74	2/1205 (0.2%)
All	All	0.51	6/9900 (0.1%)	0.76	12/13498 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	PRO	N-CD	5.29	1.55	1.47
1	A	608	PRO	N-CD	5.28	1.55	1.47
1	A	421	PRO	N-CD	5.23	1.55	1.47
3	C	111	PRO	N-CD	5.17	1.55	1.47
4	D	101	PRO	N-CD	5.13	1.55	1.47
2	B	433	PRO	N-CD	5.00	1.54	1.47

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	559	SER	C-N-CD	6.60	142.25	128.40
1	A	423	PRO	C-N-CD	6.05	141.11	128.40
1	A	632	SER	C-N-CD	5.90	140.78	128.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	422	LEU	C-N-CD	5.81	140.61	128.40
4	D	44	VAL	C-N-CD	5.79	140.57	128.40
4	D	100	THR	C-N-CD	5.75	140.47	128.40
1	A	420	GLN	C-N-CD	5.66	140.28	128.40
3	C	110	SER	C-N-CD	5.57	140.09	128.40
1	A	607	GLY	C-N-CD	5.53	140.01	128.40
1	A	560	PRO	CA-N-CD	-5.37	103.99	111.50
1	A	292	ALA	C-N-CD	5.36	139.65	128.40
2	B	432	LEU	C-N-CD	5.11	139.13	128.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	210	PHE	Peptide
1	A	256	VAL	Peptide
1	A	68	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5222	0	5113	562	0
2	B	1702	0	1793	107	0
3	C	1872	0	1911	88	0
4	D	850	0	840	50	0
5	A	238	0	214	6	0
6	A	33	0	28	0	0
7	B	43	0	60	0	0
7	C	43	0	60	1	0
All	All	10003	0	10019	772	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 39.

All (772) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:PRO:HG2	1:A:507:PHE:CD2	1.52	1.42
1:A:152:TYR:CE1	1:A:383:VAL:HG21	1.61	1.36
1:A:279:ALA:O	1:A:364:GLU:HG2	1.29	1.28
1:A:633:PRO:HB2	1:A:645:TYR:CD2	1.66	1.28
1:A:155:GLU:HG3	1:A:156:PHE:CE1	1.71	1.24
1:A:95:MET:CE	1:A:217:LEU:HD11	1.69	1.20
4:D:47:TYR:CB	4:D:50:GLN:HB2	1.72	1.19
4:D:50:GLN:OE1	4:D:54:LYS:HD2	1.43	1.19
1:A:260:LEU:HD22	1:A:312:LEU:HD22	1.23	1.17
1:A:268:THR:CG2	1:A:355:GLN:HG3	1.73	1.17
1:A:156:PHE:CD2	1:A:421:PRO:HB3	1.82	1.14
1:A:223:ALA:HB2	1:A:247:VAL:HG22	1.14	1.13
3:C:34:ILE:HD11	3:C:120:VAL:HB	1.30	1.13
4:D:47:TYR:HB2	4:D:50:GLN:CB	1.79	1.13
1:A:586:CYS:CB	1:A:620:CYS:SG	2.39	1.10
4:D:40:GLU:O	4:D:44:VAL:HG23	1.51	1.10
2:B:82:VAL:HG22	2:B:422:LEU:HD22	1.15	1.09
1:A:316:PRO:CG	1:A:507:PHE:CD2	2.35	1.09
1:A:299:VAL:O	1:A:303:VAL:HG23	1.55	1.07
1:A:604:TRP:HD1	1:A:620:CYS:SG	1.76	1.06
1:A:540:GLN:CG	1:A:606:GLN:HE21	1.68	1.05
1:A:316:PRO:HG2	1:A:507:PHE:CE2	1.92	1.05
1:A:378:MET:HE2	1:A:398:LEU:HD22	1.34	1.04
1:A:282:LEU:HD13	1:A:329:PHE:HB3	1.08	1.04
1:A:311:ALA:O	1:A:511:VAL:HG23	1.55	1.04
1:A:249:ASP:HB3	1:A:557:VAL:CG2	1.88	1.04
1:A:540:GLN:HG2	1:A:606:GLN:NE2	1.73	1.04
1:A:422:LEU:HD23	1:A:423:PRO:HD2	1.38	1.03
1:A:95:MET:HE3	1:A:217:LEU:CD1	1.87	1.02
1:A:378:MET:CE	1:A:398:LEU:HD22	1.88	1.02
1:A:152:TYR:O	1:A:154:PRO:HD3	1.60	1.02
1:A:365:LEU:H	1:A:365:LEU:HD12	1.24	1.02
1:A:432:ARG:HH12	1:A:644:GLU:HB2	1.21	1.02
1:A:378:MET:O	1:A:416:PRO:HD3	1.61	1.00
1:A:422:LEU:HD23	1:A:423:PRO:CD	1.90	1.00
1:A:95:MET:HE3	1:A:217:LEU:HD11	1.00	1.00
1:A:245:GLU:OE2	4:D:98:LEU:HD21	1.62	1.00
1:A:156:PHE:HB3	1:A:421:PRO:HB3	1.40	0.99
1:A:223:ALA:HB2	1:A:247:VAL:CG2	1.91	0.99
1:A:279:ALA:HB2	1:A:328:VAL:CG1	1.93	0.99
1:A:282:LEU:HD23	1:A:331:GLN:NE2	1.77	0.99
1:A:586:CYS:SG	1:A:620:CYS:SG	1.12	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:GLN:O	1:A:443:ASP:HB3	1.63	0.98
4:D:44:VAL:HG11	4:D:47:TYR:CD1	1.97	0.98
1:A:152:TYR:CE1	1:A:383:VAL:CG2	2.47	0.98
1:A:250:PRO:HB3	1:A:635:PHE:CD2	1.97	0.98
1:A:250:PRO:HB3	1:A:635:PHE:CE2	1.98	0.98
1:A:280:THR:OG1	1:A:305:GLN:HG2	1.63	0.97
1:A:268:THR:HG23	1:A:355:GLN:HG3	1.40	0.97
1:A:260:LEU:CD2	1:A:312:LEU:HD22	1.94	0.97
1:A:424:PRO:HA	1:A:428:GLN:NE2	1.80	0.97
2:B:429:LYS:H	2:B:429:LYS:HD2	1.30	0.96
1:A:140:CYS:HG	1:A:159:CYS:CB	1.79	0.96
1:A:147:VAL:HG11	1:A:431:LEU:HB3	1.44	0.96
1:A:223:ALA:CB	1:A:247:VAL:HG22	1.97	0.95
1:A:633:PRO:CB	1:A:645:TYR:HD2	1.78	0.95
2:B:244:TRP:CE3	2:B:247:TRP:HD1	1.84	0.95
1:A:249:ASP:HB3	1:A:557:VAL:HG21	1.48	0.94
1:A:230:CYS:SG	1:A:247:VAL:HG13	2.06	0.94
1:A:268:THR:HG21	1:A:355:GLN:HG3	1.50	0.93
1:A:224:VAL:HG21	4:D:101:PRO:HA	1.49	0.93
1:A:311:ALA:C	1:A:511:VAL:HG23	1.89	0.93
1:A:152:TYR:HE1	1:A:383:VAL:CG2	1.79	0.93
1:A:281:ARG:HH11	1:A:281:ARG:HG3	1.35	0.92
3:C:34:ILE:HD11	3:C:120:VAL:CB	1.99	0.92
1:A:152:TYR:HE1	1:A:383:VAL:HG21	1.10	0.92
1:A:139:GLN:HG2	1:A:163:GLN:HG2	1.51	0.92
3:C:90:TYR:CE2	3:C:94:LEU:HD11	2.05	0.91
1:A:279:ALA:CB	1:A:328:VAL:CG1	2.49	0.91
1:A:633:PRO:HB2	1:A:645:TYR:HD2	1.04	0.90
1:A:224:VAL:CG2	4:D:101:PRO:HA	2.02	0.89
1:A:540:GLN:HG2	1:A:606:GLN:HE21	1.33	0.89
1:A:622:ARG:HH11	1:A:622:ARG:HG2	1.35	0.89
1:A:397:LEU:CD2	1:A:439:VAL:HG23	2.02	0.89
1:A:156:PHE:CB	1:A:421:PRO:HB3	2.02	0.89
2:B:239:LYS:CG	2:B:240:TYR:CE1	2.55	0.89
1:A:300:ALA:O	1:A:304:THR:HG23	1.71	0.89
1:A:152:TYR:HD1	1:A:153:GLY:N	1.72	0.88
1:A:282:LEU:CD1	1:A:329:PHE:HB3	1.99	0.88
1:A:156:PHE:CG	1:A:421:PRO:HB3	2.08	0.88
1:A:224:VAL:HG21	4:D:100:THR:O	1.73	0.87
1:A:633:PRO:CB	1:A:645:TYR:CD2	2.51	0.87
1:A:586:CYS:SG	1:A:620:CYS:CB	2.62	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:VAL:HG22	2:B:422:LEU:CD2	2.03	0.87
1:A:249:ASP:CB	1:A:557:VAL:HG21	2.04	0.87
1:A:361:SER:OG	1:A:501:LEU:HD13	1.74	0.87
1:A:316:PRO:HG2	1:A:507:PHE:HD2	1.05	0.87
2:B:239:LYS:HG2	2:B:240:TYR:CE1	2.10	0.87
1:A:152:TYR:CZ	1:A:383:VAL:HG11	2.10	0.86
1:A:96:VAL:HG22	1:A:118:ILE:HD11	1.57	0.86
1:A:604:TRP:CD1	1:A:620:CYS:SG	2.66	0.86
1:A:162:ILE:HG21	1:A:420:GLN:OE1	1.74	0.85
1:A:156:PHE:HD2	1:A:421:PRO:HB3	1.39	0.85
1:A:371:ARG:CB	1:A:371:ARG:HH11	1.88	0.85
1:A:156:PHE:HB3	1:A:421:PRO:CB	2.06	0.85
1:A:156:PHE:CD2	1:A:421:PRO:CB	2.59	0.85
1:A:279:ALA:HB1	1:A:330:PHE:CE2	2.11	0.84
1:A:260:LEU:HD22	1:A:312:LEU:CD2	2.05	0.84
1:A:635:PHE:HZ	1:A:649:THR:HG23	1.43	0.84
1:A:155:GLU:HG3	1:A:156:PHE:CD1	2.13	0.83
1:A:378:MET:CE	1:A:398:LEU:CD2	2.55	0.83
1:A:140:CYS:SG	1:A:159:CYS:HB3	2.19	0.83
1:A:451:LYS:NZ	1:A:451:LYS:HB2	1.94	0.83
1:A:259:MET:SD	1:A:326:MET:CB	2.66	0.83
1:A:259:MET:SD	1:A:326:MET:HB2	2.19	0.83
1:A:260:LEU:CD2	1:A:312:LEU:CD2	2.56	0.83
2:B:86:PHE:CZ	2:B:419:CYS:SG	2.71	0.83
1:A:128:PRO:O	1:A:129:SER:HB2	1.78	0.83
4:D:3:LEU:HD23	4:D:40:GLU:OE1	1.79	0.82
2:B:198:VAL:HG21	4:D:94:PHE:CE1	2.14	0.82
1:A:268:THR:HG21	1:A:355:GLN:CG	2.10	0.82
1:A:563:THR:O	1:A:567:VAL:HG23	1.78	0.82
1:A:418:GLN:HE21	1:A:419:SER:H	1.28	0.82
1:A:540:GLN:HG3	1:A:606:GLN:HE21	1.42	0.82
2:B:245:THR:O	2:B:249:ILE:HG13	1.80	0.82
1:A:279:ALA:HB1	1:A:330:PHE:HE2	1.45	0.81
3:C:17:ALA:HB2	3:C:168:ILE:HG21	1.62	0.81
1:A:324:ASN:OD1	1:A:325:VAL:N	2.12	0.81
2:B:243:GLU:O	2:B:247:TRP:CD1	2.33	0.81
1:A:68:GLY:HA2	1:A:218:PHE:CD1	2.16	0.81
2:B:96:VAL:HG21	2:B:390:SER:HB3	1.62	0.81
1:A:311:ALA:O	1:A:511:VAL:CG2	2.28	0.81
1:A:279:ALA:CB	1:A:328:VAL:HG13	2.11	0.81
1:A:299:VAL:CG2	1:A:553:HIS:NE2	2.44	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:TRP:CZ3	2:B:247:TRP:HD1	2.00	0.80
1:A:586:CYS:HG	1:A:620:CYS:CB	1.91	0.80
1:A:147:VAL:CG1	1:A:431:LEU:HB3	2.12	0.80
1:A:397:LEU:HD23	1:A:439:VAL:HG23	1.64	0.80
1:A:378:MET:HE2	1:A:398:LEU:CD2	2.12	0.79
1:A:316:PRO:CG	1:A:507:PHE:HD2	1.82	0.79
1:A:68:GLY:CA	1:A:218:PHE:CE1	2.66	0.79
1:A:432:ARG:NH1	1:A:644:GLU:HB2	1.97	0.78
1:A:96:VAL:HG23	1:A:121:LEU:HB3	1.66	0.78
2:B:99:THR:HG21	2:B:181:TYR:HE1	1.49	0.78
1:A:280:THR:OG1	1:A:305:GLN:CG	2.30	0.78
1:A:245:GLU:OE2	4:D:98:LEU:CD2	2.31	0.77
2:B:244:TRP:CZ3	2:B:247:TRP:CD1	2.72	0.77
1:A:343:MET:O	1:A:347:MET:HG2	1.84	0.77
1:A:281:ARG:NH1	1:A:281:ARG:HG3	1.98	0.77
1:A:605:VAL:CG1	1:A:621:VAL:HG23	2.15	0.76
2:B:435:LEU:H	2:B:436:PRO:HD3	1.50	0.76
1:A:152:TYR:CD1	1:A:153:GLY:N	2.53	0.76
3:C:60:THR:HG21	3:C:67:LEU:HD21	1.67	0.76
1:A:269:LEU:HB3	1:A:358:ASN:HD21	1.48	0.76
2:B:237:PHE:O	2:B:241:LEU:HB2	1.85	0.76
2:B:435:LEU:CD1	2:B:439:ILE:CD1	2.64	0.76
1:A:223:ALA:CA	1:A:247:VAL:HG21	2.17	0.75
2:B:448:ALA:HB1	3:C:47:LEU:HD21	1.68	0.75
1:A:250:PRO:HA	1:A:649:THR:HG22	1.67	0.75
1:A:311:ALA:C	1:A:511:VAL:CG2	2.56	0.74
1:A:635:PHE:CZ	1:A:649:THR:HG23	2.22	0.74
2:B:239:LYS:HG3	2:B:240:TYR:CE1	2.23	0.74
1:A:279:ALA:O	1:A:364:GLU:CG	2.24	0.74
1:A:637:LEU:CB	1:A:639:GLN:HE21	2.01	0.73
4:D:47:TYR:HB2	4:D:50:GLN:HB2	0.83	0.73
1:A:637:LEU:HB3	1:A:639:GLN:HE21	1.52	0.73
1:A:64:SER:CB	1:A:219:SER:H	2.01	0.73
1:A:139:GLN:CG	1:A:163:GLN:HG2	2.18	0.73
1:A:269:LEU:HB3	1:A:358:ASN:ND2	2.04	0.73
2:B:435:LEU:N	2:B:436:PRO:CD	2.52	0.73
2:B:435:LEU:HD12	2:B:439:ILE:HG13	1.70	0.73
2:B:85:LEU:HD22	2:B:418:LEU:HD21	1.70	0.73
2:B:429:LYS:N	2:B:429:LYS:HD2	2.03	0.73
1:A:397:LEU:HG	1:A:439:VAL:HG21	1.69	0.73
1:A:282:LEU:HD13	1:A:329:PHE:CB	2.04	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:VAL:HG22	1:A:553:HIS:NE2	2.04	0.72
1:A:633:PRO:HB2	1:A:645:TYR:CE2	2.23	0.72
1:A:266:THR:HB	5:A:1714:NAG:O7	1.88	0.72
1:A:418:GLN:HE21	1:A:419:SER:N	1.87	0.72
1:A:152:TYR:C	1:A:154:PRO:HD3	2.10	0.72
2:B:241:LEU:HG	2:B:245:THR:HG22	1.70	0.72
1:A:418:GLN:CA	1:A:418:GLN:HE21	2.03	0.72
2:B:174:LEU:HG	2:B:229:ILE:HD11	1.71	0.72
1:A:422:LEU:HD23	1:A:423:PRO:N	2.03	0.72
1:A:140:CYS:SG	1:A:159:CYS:CB	2.74	0.72
1:A:418:GLN:NE2	1:A:419:SER:H	1.86	0.72
1:A:259:MET:SD	1:A:326:MET:HB3	2.30	0.71
1:A:504:GLY:O	1:A:505:THR:OG1	2.08	0.71
1:A:95:MET:CE	1:A:217:LEU:CD1	2.59	0.71
3:C:112:ILE:HD13	3:C:112:ILE:H	1.56	0.71
1:A:290:ASN:O	1:A:552:GLN:HG3	1.88	0.71
1:A:299:VAL:O	1:A:303:VAL:CG2	2.34	0.71
1:A:224:VAL:HG21	4:D:101:PRO:CA	2.20	0.71
1:A:64:SER:HB3	1:A:219:SER:H	1.56	0.70
2:B:239:LYS:CG	2:B:240:TYR:HE1	2.01	0.70
1:A:253:ASP:HB3	1:A:559:SER:O	1.91	0.70
1:A:261:LYS:O	1:A:324:ASN:ND2	2.24	0.70
1:A:451:LYS:HB2	1:A:451:LYS:HZ2	1.55	0.70
1:A:249:ASP:HB3	1:A:557:VAL:HG23	1.73	0.70
1:A:95:MET:HE2	1:A:215:MET:HE3	1.74	0.70
1:A:279:ALA:CB	1:A:330:PHE:HE2	2.05	0.70
1:A:367:GLN:O	1:A:443:ASP:CB	2.38	0.70
3:C:34:ILE:CG1	3:C:120:VAL:HG11	2.21	0.69
1:A:133:GLY:HA2	1:A:452:TYR:HE1	1.56	0.69
1:A:171:LEU:HD23	1:A:287:PHE:CE2	2.26	0.69
1:A:66:ILE:HD13	1:A:220:HIS:ND1	2.07	0.69
1:A:316:PRO:CG	1:A:507:PHE:CE2	2.72	0.69
1:A:150:ASN:O	1:A:154:PRO:HG3	1.91	0.69
1:A:424:PRO:HA	1:A:428:GLN:HE22	1.57	0.69
1:A:279:ALA:HB2	1:A:328:VAL:HG11	1.73	0.69
2:B:239:LYS:HG2	2:B:240:TYR:HE1	1.55	0.69
4:D:3:LEU:HG	4:D:11:LYS:HE2	1.75	0.69
1:A:233:ARG:O	1:A:237:GLN:HG2	1.92	0.69
1:A:278:ALA:C	1:A:305:GLN:HE22	1.97	0.69
1:A:397:LEU:CD2	1:A:439:VAL:CG2	2.71	0.69
1:A:164:TRP:CE2	1:A:423:PRO:HA	2.28	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:THR:HG23	1:A:449:HIS:CD2	2.28	0.68
1:A:95:MET:CE	1:A:215:MET:CE	2.70	0.68
1:A:94:TYR:O	1:A:118:ILE:HG13	1.94	0.68
1:A:95:MET:HG2	1:A:120:GLY:O	1.94	0.68
1:A:223:ALA:N	1:A:247:VAL:CG2	2.57	0.68
1:A:300:ALA:HB2	1:A:463:ILE:HD12	1.76	0.68
1:A:311:ALA:HB1	1:A:511:VAL:CG2	2.24	0.68
1:A:171:LEU:HD23	1:A:287:PHE:HE2	1.59	0.68
1:A:300:ALA:HB1	1:A:369:ALA:HB2	1.76	0.68
1:A:633:PRO:O	1:A:637:LEU:HD22	1.94	0.68
3:C:179:PHE:O	3:C:182:CYS:SG	2.52	0.68
1:A:223:ALA:CA	1:A:247:VAL:CG2	2.72	0.68
1:A:256:VAL:HG22	1:A:329:PHE:HB2	1.76	0.68
1:A:141:PRO:HG2	1:A:424:PRO:HG3	1.75	0.68
1:A:111:LEU:HD21	1:A:118:ILE:HD13	1.76	0.67
1:A:96:VAL:HG23	1:A:121:LEU:CB	2.24	0.67
1:A:68:GLY:N	1:A:218:PHE:CD1	2.62	0.67
1:A:311:ALA:HB1	1:A:511:VAL:HG22	1.76	0.67
1:A:95:MET:CE	1:A:215:MET:HE2	2.24	0.67
1:A:281:ARG:HB2	1:A:333:GLU:HB2	1.75	0.67
1:A:68:GLY:N	1:A:218:PHE:CE1	2.63	0.67
1:A:453:TYR:O	1:A:454:GLN:C	2.32	0.67
2:B:182:LEU:HD21	2:B:201:LEU:HD23	1.76	0.67
1:A:54:LEU:HD12	1:A:248:CYS:SG	2.35	0.67
2:B:435:LEU:HD11	2:B:439:ILE:CD1	2.24	0.67
3:C:163:LEU:HD11	3:C:217:ILE:HD13	1.75	0.67
1:A:256:VAL:HG21	1:A:567:VAL:HG12	1.77	0.67
1:A:605:VAL:HG11	1:A:621:VAL:CG2	2.24	0.67
1:A:72:VAL:HG13	1:A:94:TYR:CD1	2.29	0.67
1:A:64:SER:N	1:A:219:SER:O	2.28	0.67
1:A:224:VAL:HG11	4:D:99:GLY:O	1.94	0.66
2:B:435:LEU:CD1	2:B:439:ILE:HD11	2.26	0.66
1:A:223:ALA:HA	1:A:247:VAL:HG21	1.77	0.66
3:C:34:ILE:CD1	3:C:120:VAL:HB	2.18	0.66
1:A:64:SER:HB3	1:A:219:SER:C	2.15	0.66
1:A:299:VAL:HG11	1:A:526:LEU:HD21	1.76	0.66
1:A:529:ALA:HB2	1:A:551:LEU:CD1	2.24	0.66
1:A:68:GLY:CA	1:A:218:PHE:CD1	2.77	0.66
1:A:369:ALA:HB2	1:A:463:ILE:HD11	1.77	0.66
1:A:282:LEU:HD23	1:A:331:GLN:HE21	1.61	0.66
1:A:378:MET:O	1:A:416:PRO:CD	2.43	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:SER:CB	1:A:560:PRO:HD3	2.25	0.66
3:C:163:LEU:HD21	3:C:204:THR:HG22	1.76	0.66
1:A:305:GLN:HB2	1:A:365:LEU:HD11	1.78	0.65
1:A:249:ASP:OD1	1:A:652:ARG:NH2	2.29	0.65
1:A:171:LEU:CD2	1:A:287:PHE:HE2	2.09	0.65
1:A:385:GLN:HB3	1:A:391:ARG:HD3	1.78	0.65
3:C:112:ILE:HG12	3:C:117:MET:HG3	1.76	0.65
1:A:68:GLY:HA2	1:A:218:PHE:CE1	2.31	0.65
2:B:85:LEU:CD1	2:B:422:LEU:HD11	2.27	0.65
1:A:162:ILE:HD12	1:A:164:TRP:CH2	2.33	0.64
1:A:397:LEU:HD21	1:A:439:VAL:HG23	1.78	0.64
1:A:162:ILE:HD11	1:A:164:TRP:CZ2	2.32	0.64
2:B:435:LEU:H	2:B:436:PRO:CD	2.09	0.64
1:A:418:GLN:HA	1:A:418:GLN:HE21	1.63	0.64
1:A:434:ARG:O	1:A:435:ASN:HB2	1.95	0.64
1:A:68:GLY:CA	1:A:218:PHE:HE1	2.08	0.64
1:A:95:MET:HE2	1:A:215:MET:CE	2.28	0.64
1:A:365:LEU:HD12	1:A:365:LEU:N	2.03	0.64
1:A:378:MET:HE3	1:A:398:LEU:CD2	2.27	0.64
1:A:579:VAL:HG12	1:A:620:CYS:O	1.98	0.64
2:B:249:ILE:O	2:B:253:ILE:HG22	1.97	0.64
3:C:112:ILE:H	3:C:112:ILE:CD1	2.10	0.64
1:A:223:ALA:CB	1:A:247:VAL:CG2	2.64	0.64
3:C:159:THR:HG21	3:C:210:TYR:CD1	2.33	0.64
3:C:112:ILE:CG1	3:C:117:MET:HG3	2.28	0.63
1:A:499:TYR:O	1:A:503:GLY:N	2.31	0.63
1:A:156:PHE:HD2	1:A:421:PRO:CB	2.05	0.63
1:A:185:ASP:OD1	1:A:187:ASN:N	2.29	0.63
1:A:260:LEU:HD21	1:A:312:LEU:CD2	2.27	0.63
1:A:559:SER:HB2	1:A:560:PRO:HD3	1.79	0.63
1:A:576:GLY:HA3	1:A:623:SER:HB3	1.81	0.63
1:A:622:ARG:NH1	1:A:622:ARG:HG2	2.04	0.63
1:A:260:LEU:HD12	1:A:313:GLN:HE22	1.63	0.62
1:A:524:GLY:HA2	1:A:531:ASN:HD21	1.64	0.62
1:A:268:THR:HG21	1:A:355:GLN:OE1	1.99	0.62
1:A:95:MET:CG	1:A:120:GLY:O	2.47	0.62
2:B:100:ILE:HD11	2:B:238:ILE:HD13	1.81	0.62
1:A:500:GLU:O	1:A:503:GLY:HA2	1.98	0.62
1:A:378:MET:HE3	1:A:398:LEU:HD23	1.82	0.62
2:B:99:THR:HG21	2:B:181:TYR:CE1	2.34	0.62
1:A:268:THR:HG21	1:A:355:GLN:CD	2.21	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:61:ASP:O	3:C:62:ARG:HB2	1.98	0.62
1:A:605:VAL:HG22	1:A:606:GLN:O	2.00	0.61
1:A:249:ASP:OD1	1:A:652:ARG:NE	2.33	0.61
1:A:150:ASN:ND2	1:A:150:ASN:H	1.98	0.61
1:A:95:MET:SD	1:A:217:LEU:HD11	2.39	0.61
1:A:305:GLN:HB2	1:A:365:LEU:CD1	2.30	0.61
1:A:371:ARG:HB3	1:A:371:ARG:HH11	1.63	0.61
1:A:385:GLN:CA	1:A:391:ARG:HD3	2.30	0.61
1:A:152:TYR:CD1	1:A:383:VAL:HG21	2.27	0.61
1:A:422:LEU:CD2	1:A:423:PRO:HD2	2.22	0.61
1:A:511:VAL:O	1:A:511:VAL:HG13	2.01	0.61
2:B:85:LEU:HD13	2:B:422:LEU:HD11	1.82	0.61
2:B:424:LEU:O	2:B:428:PHE:HB2	2.00	0.61
1:A:337:TYR:HB3	1:A:429:ARG:HG3	1.83	0.60
2:B:207:VAL:CG1	4:D:26:LEU:HD21	2.31	0.60
1:A:155:GLU:CG	1:A:156:PHE:CE1	2.65	0.60
1:A:54:LEU:HD23	1:A:59:GLN:HB2	1.82	0.60
1:A:300:ALA:HB2	1:A:463:ILE:CD1	2.31	0.60
1:A:605:VAL:HG11	1:A:621:VAL:HG23	1.80	0.60
1:A:341:SER:CB	1:A:429:ARG:HH11	2.14	0.60
2:B:241:LEU:CD1	2:B:245:THR:HG21	2.31	0.60
1:A:260:LEU:CD1	1:A:313:GLN:NE2	2.64	0.60
1:A:371:ARG:CG	1:A:371:ARG:HH11	2.13	0.60
2:B:247:TRP:CE3	2:B:247:TRP:HA	2.36	0.60
1:A:66:ILE:HD13	1:A:220:HIS:CE1	2.36	0.60
1:A:96:VAL:CG2	1:A:121:LEU:HB3	2.32	0.60
1:A:304:THR:HG22	1:A:487:LEU:HG	1.83	0.60
1:A:98:LEU:HD13	1:A:107:LEU:HD21	1.84	0.60
1:A:260:LEU:HD12	1:A:313:GLN:NE2	2.17	0.60
1:A:133:GLY:HA2	1:A:452:TYR:CE1	2.35	0.60
2:B:435:LEU:HD12	2:B:439:ILE:CD1	2.32	0.60
4:D:45:PRO:HG2	4:D:46:ALA:H	1.66	0.60
2:B:244:TRP:CE3	2:B:247:TRP:CD1	2.76	0.60
1:A:51:VAL:HG22	1:A:221:MET:HE1	1.84	0.59
1:A:97:LEU:HD13	1:A:192:ILE:HG21	1.84	0.59
3:C:112:ILE:HD13	3:C:112:ILE:O	2.02	0.59
1:A:66:ILE:HB	1:A:220:HIS:CE1	2.37	0.59
2:B:86:PHE:HZ	2:B:419:CYS:SG	2.21	0.59
3:C:159:THR:HG21	3:C:210:TYR:CE1	2.38	0.59
1:A:463:ILE:HG23	1:A:465:VAL:HG23	1.84	0.59
1:A:385:GLN:HB3	1:A:391:ARG:CD	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ILE:CD1	1:A:164:TRP:CZ2	2.85	0.59
3:C:163:LEU:HD13	3:C:214:LEU:HD12	1.84	0.59
1:A:341:SER:HB2	1:A:429:ARG:HD2	1.85	0.58
1:A:101:LYS:CG	1:A:126:THR:HG21	2.33	0.58
1:A:313:GLN:HG2	1:A:575:THR:O	2.03	0.58
1:A:279:ALA:HB1	1:A:328:VAL:HG13	1.85	0.58
2:B:96:VAL:HG21	2:B:390:SER:CB	2.34	0.58
1:A:148:TYR:HE2	1:A:422:LEU:N	2.01	0.58
1:A:529:ALA:HB2	1:A:551:LEU:HD11	1.84	0.58
2:B:239:LYS:HG3	2:B:240:TYR:CD1	2.37	0.58
4:D:48:THR:OG1	4:D:49:GLU:HG2	2.03	0.58
1:A:250:PRO:HB3	1:A:635:PHE:HE2	1.66	0.58
4:D:51:SER:O	4:D:54:LYS:HG2	2.04	0.58
3:C:114:ILE:HD12	3:C:114:ILE:O	2.03	0.58
1:A:148:TYR:HE2	1:A:422:LEU:H	1.50	0.58
1:A:250:PRO:CB	1:A:635:PHE:CE2	2.83	0.57
1:A:295:ALA:O	1:A:300:ALA:N	2.34	0.57
1:A:434:ARG:HH11	1:A:434:ARG:CG	2.15	0.57
1:A:586:CYS:SG	1:A:604:TRP:HD1	2.26	0.57
1:A:559:SER:OG	1:A:560:PRO:HD3	2.04	0.57
1:A:96:VAL:CG2	1:A:118:ILE:HD11	2.31	0.57
1:A:123:VAL:HG23	1:A:123:VAL:O	2.03	0.57
1:A:430:PHE:HB3	1:A:436:ILE:HD11	1.87	0.57
3:C:30:LEU:O	3:C:34:ILE:HG23	2.04	0.57
4:D:40:GLU:O	4:D:44:VAL:CG2	2.41	0.57
3:C:34:ILE:CG1	3:C:120:VAL:CG1	2.83	0.57
1:A:186:GLU:OE1	1:A:189:THR:OG1	2.21	0.57
4:D:39:ARG:O	4:D:43:LEU:HB2	2.05	0.57
1:A:304:THR:OG1	1:A:365:LEU:HD22	2.05	0.56
1:A:156:PHE:HD2	1:A:421:PRO:CD	2.18	0.56
2:B:241:LEU:HG	2:B:245:THR:CG2	2.34	0.56
1:A:279:ALA:HB2	1:A:328:VAL:HG12	1.85	0.56
1:A:418:GLN:HA	1:A:418:GLN:NE2	2.20	0.56
2:B:435:LEU:HD11	2:B:439:ILE:HD12	1.86	0.56
2:B:435:LEU:HD12	2:B:439:ILE:CG1	2.35	0.56
1:A:97:LEU:CD1	1:A:192:ILE:HG21	2.36	0.56
2:B:244:TRP:CE3	2:B:244:TRP:HA	2.41	0.56
1:A:605:VAL:CG2	1:A:606:GLN:N	2.68	0.56
3:C:34:ILE:HD11	3:C:120:VAL:CG1	2.35	0.56
1:A:335:PHE:O	1:A:337:TYR:N	2.38	0.56
2:B:85:LEU:HD13	2:B:422:LEU:CD1	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ALA:O	1:A:305:GLN:NE2	2.39	0.56
1:A:364:GLU:OE1	1:A:426:SER:N	2.38	0.56
1:A:156:PHE:CD2	1:A:421:PRO:CA	2.89	0.56
2:B:247:TRP:HE3	2:B:247:TRP:HA	1.71	0.56
1:A:222:HIS:O	1:A:651:SER:OG	2.23	0.55
1:A:296:GLU:OE1	1:A:450:ASN:HB2	2.05	0.55
1:A:95:MET:CE	1:A:217:LEU:HD21	2.36	0.55
1:A:101:LYS:HD3	1:A:126:THR:HG21	1.88	0.55
4:D:96:ILE:HG22	4:D:97:PRO:HD2	1.88	0.55
1:A:171:LEU:CG	1:A:287:PHE:HE2	2.19	0.55
1:A:516:GLN:O	1:A:519:THR:HG22	2.05	0.55
1:A:339:GLY:HA2	1:A:630:ALA:HB1	1.87	0.55
1:A:223:ALA:O	1:A:224:VAL:HG13	2.07	0.55
1:A:434:ARG:HG2	1:A:434:ARG:NH1	2.20	0.55
1:A:233:ARG:HB2	4:D:96:ILE:CD1	2.36	0.55
1:A:397:LEU:HD13	1:A:501:LEU:HD11	1.88	0.55
1:A:450:ASN:OD1	1:A:453:TYR:HA	2.07	0.55
1:A:633:PRO:CG	1:A:645:TYR:CD2	2.89	0.55
1:A:586:CYS:HG	1:A:604:TRP:HD1	1.54	0.55
3:C:34:ILE:HG13	3:C:120:VAL:CG1	2.37	0.55
1:A:299:VAL:HG11	1:A:526:LEU:CD2	2.37	0.55
1:A:54:LEU:CD2	1:A:59:GLN:HB2	2.37	0.55
2:B:241:LEU:CD1	2:B:245:THR:CG2	2.86	0.54
3:C:111:PRO:HG2	3:C:112:ILE:HD12	1.90	0.54
1:A:294:GLY:HA3	1:A:553:HIS:HD2	1.72	0.54
1:A:605:VAL:HG23	1:A:606:GLN:N	2.22	0.54
3:C:62:ARG:HG2	3:C:68:GLN:OE1	2.07	0.54
1:A:385:GLN:O	1:A:391:ARG:HB2	2.07	0.54
1:A:540:GLN:HG2	1:A:606:GLN:HE22	1.67	0.54
2:B:408:ILE:HD13	3:C:131:VAL:HG11	1.90	0.54
1:A:224:VAL:HG21	4:D:100:THR:C	2.28	0.54
1:A:347:MET:SD	1:A:352:PHE:CE2	3.01	0.54
1:A:281:ARG:HH11	1:A:281:ARG:CG	2.13	0.54
1:A:260:LEU:CD1	1:A:313:GLN:HE22	2.20	0.54
1:A:369:ALA:HB1	1:A:463:ILE:CG1	2.38	0.54
1:A:422:LEU:HD22	1:A:423:PRO:O	2.07	0.54
1:A:337:TYR:OH	1:A:428:GLN:NE2	2.41	0.54
1:A:559:SER:CB	1:A:560:PRO:CD	2.86	0.53
3:C:90:TYR:HE2	3:C:121:SER:HB2	1.74	0.53
1:A:156:PHE:HD2	1:A:421:PRO:HD3	1.72	0.53
1:A:552:GLN:OE1	1:A:552:GLN:HA	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:ALA:CB	1:A:551:LEU:HD11	2.38	0.53
3:C:40:PHE:O	3:C:44:VAL:HG23	2.09	0.53
1:A:506:ASN:O	1:A:507:PHE:HD1	1.91	0.53
1:A:222:HIS:O	1:A:223:ALA:HB3	2.09	0.53
4:D:31:LEU:HD13	4:D:64:PHE:CZ	2.43	0.53
1:A:289:TRP:NE1	1:A:650:GLU:OE2	2.40	0.53
1:A:341:SER:HB2	1:A:429:ARG:HH11	1.73	0.53
1:A:152:TYR:CE1	1:A:383:VAL:CB	2.91	0.53
1:A:385:GLN:CB	1:A:391:ARG:HD3	2.39	0.53
2:B:241:LEU:HD11	2:B:245:THR:HG21	1.91	0.53
5:A:1706:NAG:O3	5:A:1707:NAG:H83	2.09	0.53
1:A:200:ASN:HD21	1:A:213:CYS:HB3	1.74	0.53
1:A:288:PHE:CE2	1:A:456:ILE:HD11	2.44	0.53
1:A:633:PRO:CG	1:A:645:TYR:HD2	2.20	0.53
1:A:443:ASP:OD1	1:A:444:HIS:ND1	2.41	0.52
1:A:164:TRP:CZ2	1:A:423:PRO:HA	2.43	0.52
2:B:242:PRO:HD2	2:B:245:THR:HB	1.90	0.52
1:A:369:ALA:CB	1:A:463:ILE:HD11	2.39	0.52
1:A:40:ILE:HD11	3:C:157:PHE:HZ	1.74	0.52
1:A:268:THR:CG2	1:A:355:GLN:CG	2.60	0.52
3:C:34:ILE:HG12	3:C:120:VAL:HG11	1.91	0.52
1:A:82:LEU:HD23	1:A:110:LYS:NZ	2.25	0.52
3:C:34:ILE:HB	3:C:90:TYR:OH	2.09	0.52
1:A:68:GLY:HA2	1:A:218:PHE:HD1	1.74	0.52
3:C:126:GLY:O	3:C:168:ILE:HG12	2.09	0.52
3:C:137:ILE:HD11	3:C:160:SER:OG	2.10	0.52
1:A:104:THR:HG22	1:A:105:ARG:H	1.75	0.52
1:A:645:TYR:O	1:A:646:SER:OG	2.23	0.52
1:A:155:GLU:CG	1:A:156:PHE:CD1	2.89	0.52
1:A:182:LEU:HD13	1:A:288:PHE:CE2	2.44	0.52
1:A:162:ILE:CG2	1:A:420:GLN:OE1	2.55	0.52
2:B:241:LEU:CG	2:B:245:THR:HG22	2.38	0.52
1:A:91:ASN:O	1:A:93:PRO:HD2	2.10	0.51
1:A:162:ILE:O	1:A:163:GLN:HB2	2.08	0.51
1:A:40:ILE:HD11	3:C:157:PHE:CZ	2.45	0.51
1:A:64:SER:HB3	1:A:219:SER:N	2.23	0.51
1:A:66:ILE:HB	1:A:220:HIS:NE2	2.26	0.51
1:A:326:MET:HG3	1:A:326:MET:O	2.09	0.51
2:B:106:TYR:CG	2:B:235:LEU:HD22	2.45	0.51
3:C:106:GLU:HA	3:C:106:GLU:OE1	2.10	0.51
4:D:97:PRO:HG2	4:D:100:THR:OG1	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:LEU:HD13	1:A:358:ASN:HD22	1.76	0.51
1:A:443:ASP:OD1	1:A:444:HIS:N	2.43	0.51
1:A:605:VAL:HG11	1:A:621:VAL:HG21	1.92	0.51
2:B:435:LEU:CD1	2:B:439:ILE:HD12	2.41	0.51
1:A:249:ASP:OD1	1:A:652:ARG:CZ	2.59	0.51
1:A:562:ASN:N	1:A:562:ASN:OD1	2.43	0.51
1:A:224:VAL:CG1	4:D:99:GLY:O	2.58	0.51
1:A:372:THR:CG2	1:A:449:HIS:CD2	2.93	0.51
3:C:170:LEU:HG	3:C:174:TRP:CZ2	2.46	0.51
3:C:90:TYR:CE2	3:C:94:LEU:CD1	2.87	0.51
4:D:44:VAL:CG1	4:D:47:TYR:CD1	2.86	0.51
1:A:390:VAL:CG2	5:A:1705:NAG:H82	2.41	0.51
1:A:280:THR:CG2	1:A:365:LEU:HD13	2.41	0.51
2:B:250:LEU:O	2:B:439:ILE:HG21	2.10	0.51
1:A:343:MET:CE	1:A:347:MET:SD	2.98	0.51
1:A:559:SER:HB2	1:A:560:PRO:CD	2.40	0.51
1:A:60:ILE:HG12	1:A:648:TRP:CZ3	2.46	0.51
1:A:102:HIS:O	1:A:107:LEU:HD23	2.11	0.50
1:A:283:ASP:HA	1:A:553:HIS:HB3	1.93	0.50
1:A:425:SER:O	1:A:428:GLN:N	2.44	0.50
1:A:635:PHE:CZ	1:A:649:THR:CG2	2.93	0.50
1:A:693:LYS:NZ	3:C:242:SER:O	2.44	0.50
1:A:364:GLU:O	1:A:440:VAL:HA	2.11	0.50
2:B:402:GLY:O	2:B:404:TRP:N	2.44	0.50
2:B:448:ALA:CB	3:C:47:LEU:HD21	2.40	0.50
1:A:633:PRO:CB	1:A:645:TYR:CE2	2.89	0.50
1:A:95:MET:SD	1:A:215:MET:HE2	2.52	0.50
2:B:416:ILE:CD1	3:C:40:PHE:HB2	2.42	0.50
2:B:82:VAL:HB	3:C:33:ILE:HD11	1.93	0.50
1:A:540:GLN:CG	1:A:606:GLN:NE2	2.39	0.50
1:A:633:PRO:HD2	1:A:645:TYR:CD2	2.47	0.50
2:B:240:TYR:CD1	2:B:240:TYR:N	2.77	0.50
1:A:145:PHE:CG	1:A:336:ASP:HB3	2.47	0.50
1:A:506:ASN:C	1:A:507:PHE:CD1	2.85	0.50
2:B:435:LEU:HD11	2:B:439:ILE:HD11	1.89	0.50
1:A:162:ILE:CD1	1:A:164:TRP:CH2	2.95	0.50
1:A:270:LYS:HG3	1:A:271:PRO:CD	2.42	0.50
1:A:171:LEU:HG	1:A:287:PHE:HE2	1.75	0.50
1:A:631:LEU:HD23	1:A:635:PHE:HB2	1.94	0.50
2:B:253:ILE:HD13	2:B:388:PHE:CZ	2.46	0.50
1:A:622:ARG:CG	1:A:622:ARG:NH1	2.73	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:TYR:CZ	1:A:383:VAL:CG1	2.89	0.49
1:A:58:HIS:N	1:A:58:HIS:ND1	2.60	0.49
1:A:633:PRO:CD	1:A:645:TYR:HD2	2.25	0.49
1:A:223:ALA:N	1:A:247:VAL:HG21	2.25	0.49
1:A:250:PRO:HB3	1:A:635:PHE:HD2	1.64	0.49
1:A:557:VAL:HG13	1:A:558:SER:N	2.26	0.49
1:A:230:CYS:SG	1:A:247:VAL:CG1	2.91	0.49
1:A:280:THR:HG23	1:A:365:LEU:HD13	1.93	0.49
1:A:68:GLY:H	1:A:218:PHE:HD1	1.55	0.49
2:B:244:TRP:O	2:B:248:LEU:N	2.34	0.49
4:D:96:ILE:CG2	4:D:97:PRO:HD2	2.42	0.49
1:A:605:VAL:CG2	1:A:606:GLN:O	2.61	0.49
1:A:49:PRO:HD3	1:A:656:ILE:HD13	1.93	0.49
2:B:466:TYR:CZ	3:C:163:LEU:HD23	2.47	0.49
3:C:24:THR:HG21	3:C:119:TYR:CE1	2.47	0.49
3:C:42:TRP:CH2	3:C:46:LEU:HD12	2.47	0.49
1:A:152:TYR:C	1:A:152:TYR:CD1	2.86	0.49
1:A:152:TYR:CE1	1:A:383:VAL:HG11	2.47	0.49
1:A:418:GLN:CA	1:A:418:GLN:NE2	2.73	0.49
3:C:10:THR:CB	3:C:138:LEU:HD21	2.43	0.49
3:C:80:VAL:HG11	3:C:198:LEU:HD12	1.94	0.49
3:C:122:GLY:HA3	3:C:172:THR:HA	1.94	0.49
1:A:385:GLN:HA	1:A:391:ARG:HB2	1.93	0.49
1:A:82:LEU:HD23	1:A:110:LYS:HZ2	1.78	0.49
3:C:227:TRP:O	3:C:231:THR:HG23	2.13	0.49
1:A:152:TYR:O	1:A:154:PRO:CD	2.47	0.49
1:A:222:HIS:CD2	1:A:222:HIS:N	2.78	0.49
1:A:274:ARG:HD2	1:A:360:ASP:OD2	2.13	0.49
1:A:74:HIS:N	1:A:95:MET:O	2.45	0.49
2:B:211:ILE:O	2:B:215:TRP:N	2.45	0.49
1:A:222:HIS:HB3	1:A:247:VAL:HG23	1.95	0.49
1:A:72:VAL:HG13	1:A:94:TYR:CE1	2.48	0.49
1:A:378:MET:SD	1:A:413:LEU:CD2	3.01	0.48
2:B:385:ASP:OD1	2:B:435:LEU:HD22	2.12	0.48
1:A:121:LEU:O	1:A:180:ILE:HA	2.13	0.48
1:A:224:VAL:O	1:A:225:ILE:HB	2.13	0.48
2:B:250:LEU:HD13	2:B:392:LEU:HD12	1.93	0.48
1:A:101:LYS:CD	1:A:126:THR:HG21	2.42	0.48
1:A:365:LEU:CD1	1:A:365:LEU:H	2.08	0.48
1:A:152:TYR:OH	1:A:383:VAL:HB	2.13	0.48
1:A:57:THR:HG22	1:A:58:HIS:ND1	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:ARG:CZ	1:A:631:LEU:HD12	2.43	0.48
3:C:80:VAL:CG1	3:C:198:LEU:HD12	2.43	0.48
3:C:115:ARG:CB	3:C:115:ARG:HH11	2.27	0.48
2:B:182:LEU:HD22	2:B:202:ILE:CD1	2.44	0.48
2:B:239:LYS:CG	2:B:240:TYR:CD1	2.93	0.48
1:A:186:GLU:HA	1:A:186:GLU:OE1	2.13	0.48
1:A:311:ALA:CA	1:A:511:VAL:HG23	2.44	0.48
2:B:387:ILE:O	2:B:391:VAL:HG23	2.13	0.48
1:A:290:ASN:O	1:A:552:GLN:CG	2.59	0.48
1:A:419:SER:OG	1:A:419:SER:O	2.30	0.47
1:A:609:LEU:CD2	1:A:614:THR:HA	2.44	0.47
2:B:91:LEU:O	2:B:95:VAL:HG23	2.14	0.47
3:C:206:LEU:HD23	3:C:212:ALA:HB1	1.95	0.47
3:C:62:ARG:CG	3:C:68:GLN:OE1	2.61	0.47
1:A:294:GLY:O	1:A:299:VAL:HG23	2.14	0.47
1:A:269:LEU:CD1	1:A:358:ASN:HD22	2.27	0.47
1:A:341:SER:OG	1:A:429:ARG:NH1	2.47	0.47
1:A:679:ILE:HG21	3:C:12:VAL:HA	1.96	0.47
1:A:385:GLN:O	1:A:391:ARG:HD3	2.14	0.47
1:A:451:LYS:HB2	1:A:451:LYS:HZ3	1.76	0.47
3:C:61:ASP:O	3:C:62:ARG:CB	2.63	0.47
4:D:39:ARG:O	4:D:43:LEU:CB	2.62	0.47
1:A:122:ALA:HA	1:A:181:PHE:O	2.15	0.47
1:A:432:ARG:HH12	1:A:644:GLU:CB	2.09	0.47
1:A:60:ILE:HG22	1:A:173:TYR:O	2.15	0.47
1:A:371:ARG:HD3	1:A:376:LEU:CD1	2.45	0.47
4:D:47:TYR:CB	4:D:50:GLN:CB	2.63	0.47
1:A:552:GLN:HG2	5:A:1710:NAG:C8	2.45	0.47
1:A:349:LYS:HB3	1:A:351:LYS:HD2	1.97	0.47
1:A:369:ALA:CB	1:A:463:ILE:CG1	2.92	0.47
1:A:427:LEU:O	1:A:427:LEU:HD12	2.15	0.47
1:A:369:ALA:CB	1:A:463:ILE:HG13	2.45	0.47
1:A:66:ILE:CD1	1:A:220:HIS:ND1	2.76	0.47
1:A:98:LEU:CD1	1:A:107:LEU:HD21	2.45	0.47
2:B:208:VAL:O	2:B:211:ILE:HG13	2.15	0.47
2:B:208:VAL:HG21	4:D:28:PHE:CD1	2.50	0.47
1:A:633:PRO:HD2	1:A:645:TYR:HD2	1.80	0.47
2:B:211:ILE:HD12	2:B:212:SER:N	2.30	0.47
3:C:112:ILE:N	3:C:112:ILE:CD1	2.73	0.47
1:A:68:GLY:HA3	1:A:218:PHE:HE1	1.81	0.46
1:A:304:THR:OG1	1:A:365:LEU:CD2	2.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:TRP:HB3	1:A:448:PHE:CE1	2.50	0.46
1:A:269:LEU:HD23	1:A:269:LEU:HA	1.79	0.46
3:C:90:TYR:CE2	3:C:121:SER:HB2	2.50	0.46
3:C:174:TRP:CZ2	3:C:197:HIS:HA	2.50	0.46
1:A:503:GLY:O	1:A:505:THR:HG23	2.15	0.46
1:A:76:VAL:HB	1:A:98:LEU:HD23	1.98	0.46
1:A:253:ASP:O	1:A:630:ALA:HB3	2.16	0.46
1:A:377:TRP:CE3	1:A:415:ARG:O	2.69	0.46
2:B:80:LYS:O	2:B:83:ILE:HG22	2.15	0.46
1:A:343:MET:HE2	1:A:347:MET:SD	2.56	0.46
1:A:53:LEU:HD21	1:A:554:TYR:OH	2.16	0.46
1:A:63:GLN:HG3	1:A:221:MET:HB2	1.98	0.46
4:D:3:LEU:O	4:D:11:LYS:HE2	2.16	0.46
2:B:207:VAL:HG11	4:D:26:LEU:HD21	1.97	0.46
1:A:281:ARG:HD3	1:A:297:SER:O	2.15	0.46
1:A:152:TYR:OH	1:A:383:VAL:CG1	2.64	0.46
4:D:97:PRO:HB2	4:D:100:THR:OG1	2.15	0.46
1:A:233:ARG:HB2	4:D:96:ILE:HD13	1.97	0.45
2:B:241:LEU:HD11	2:B:245:THR:CG2	2.46	0.45
4:D:44:VAL:HG11	4:D:47:TYR:HD1	1.66	0.45
1:A:306:LEU:HD23	1:A:306:LEU:O	2.17	0.45
1:A:285:ARG:HG2	1:A:334:THR:OG1	2.16	0.45
1:A:268:THR:HA	1:A:353:PRO:HA	1.97	0.45
2:B:234:ALA:HA	2:B:391:VAL:HG22	1.98	0.45
1:A:300:ALA:CB	1:A:369:ALA:HB2	2.44	0.45
1:A:275:VAL:HG12	1:A:324:ASN:HB3	1.98	0.45
1:A:253:ASP:OD1	1:A:555:ILE:HG23	2.17	0.45
1:A:253:ASP:CB	1:A:559:SER:O	2.61	0.45
1:A:644:GLU:HG2	1:A:645:TYR:HD1	1.80	0.45
1:A:397:LEU:HD21	1:A:439:VAL:CG2	2.42	0.45
1:A:128:PRO:O	1:A:129:SER:CB	2.56	0.45
1:A:279:ALA:CA	1:A:328:VAL:HG13	2.46	0.45
1:A:367:GLN:HE21	1:A:367:GLN:HB3	1.58	0.45
3:C:106:GLU:O	3:C:107:ASP:HB2	2.15	0.45
4:D:31:LEU:HD13	4:D:64:PHE:CE2	2.52	0.45
1:A:95:MET:HE1	1:A:217:LEU:HD21	1.97	0.45
1:A:223:ALA:HB1	1:A:230:CYS:SG	2.57	0.45
1:A:583:ARG:HB2	1:A:604:TRP:CZ2	2.51	0.45
3:C:34:ILE:HG13	3:C:120:VAL:HG12	1.98	0.45
1:A:157:ALA:O	1:A:158:HIS:ND1	2.50	0.45
1:A:164:TRP:CZ2	1:A:423:PRO:CA	3.00	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:MET:HE1	1:A:215:MET:CE	2.47	0.45
1:A:280:THR:OG1	1:A:305:GLN:CB	2.64	0.45
1:A:341:SER:HB2	1:A:429:ARG:NH1	2.32	0.45
1:A:431:LEU:HD12	1:A:431:LEU:HA	1.83	0.45
1:A:96:VAL:O	1:A:121:LEU:HB2	2.17	0.45
1:A:283:ASP:OD2	1:A:555:ILE:HD11	2.17	0.44
1:A:57:THR:CG2	1:A:58:HIS:CE1	3.00	0.44
4:D:44:VAL:HG12	4:D:46:ALA:O	2.17	0.44
1:A:634:ALA:HB2	1:A:645:TYR:HB2	2.00	0.44
1:A:637:LEU:CB	1:A:639:GLN:HG2	2.47	0.44
1:A:156:PHE:CD2	1:A:421:PRO:HD3	2.52	0.44
1:A:311:ALA:CB	1:A:511:VAL:CG2	2.95	0.44
2:B:83:ILE:HG21	3:C:29:PRO:HB3	1.99	0.44
3:C:34:ILE:HG13	3:C:35:LEU:N	2.32	0.44
1:A:371:ARG:NH1	1:A:371:ARG:CG	2.73	0.44
1:A:397:LEU:CG	1:A:439:VAL:HG21	2.43	0.44
1:A:498:LEU:O	1:A:502:ALA:N	2.32	0.44
2:B:248:LEU:HD23	2:B:248:LEU:HA	1.81	0.44
2:B:92:CYS:O	2:B:96:VAL:HG23	2.17	0.44
3:C:12:VAL:O	3:C:165:ALA:HB2	2.18	0.44
1:A:95:MET:CE	1:A:215:MET:HE3	2.39	0.44
1:A:377:TRP:HA	1:A:414:ARG:O	2.17	0.44
2:B:416:ILE:CD1	3:C:36:VAL:HG12	2.48	0.44
1:A:264:ASN:O	1:A:265:THR:CB	2.66	0.44
1:A:586:CYS:HB2	1:A:620:CYS:SG	2.46	0.44
2:B:85:LEU:HD21	2:B:381:LEU:HD23	1.98	0.44
1:A:182:LEU:HD23	1:A:184:GLU:HG3	1.99	0.44
1:A:425:SER:O	1:A:426:SER:C	2.56	0.44
3:C:42:TRP:CZ3	3:C:46:LEU:HD12	2.52	0.44
1:A:139:GLN:HG2	1:A:163:GLN:CG	2.35	0.44
1:A:284:SER:OG	1:A:553:HIS:HB2	2.17	0.44
1:A:68:GLY:N	1:A:218:PHE:HD1	2.11	0.44
1:A:95:MET:HG3	1:A:120:GLY:O	2.17	0.43
1:A:632:SER:HB3	1:A:645:TYR:O	2.17	0.43
2:B:250:LEU:CD1	2:B:392:LEU:HG	2.48	0.43
1:A:185:ASP:HB3	1:A:188:GLU:OE2	2.18	0.43
1:A:298:ALA:O	1:A:302:PHE:CD2	2.71	0.43
3:C:90:TYR:HE2	3:C:94:LEU:HD11	1.72	0.43
4:D:97:PRO:HG2	4:D:100:THR:HG1	1.83	0.43
1:A:103:PHE:CG	1:A:103:PHE:O	2.70	0.43
1:A:337:TYR:CB	1:A:429:ARG:HG3	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:LEU:HD12	1:A:494:LEU:HD12	2.00	0.43
2:B:416:ILE:HD11	3:C:36:VAL:HG12	1.98	0.43
3:C:80:VAL:HG13	3:C:197:HIS:CG	2.54	0.43
3:C:7:PHE:O	3:C:10:THR:HG22	2.19	0.43
4:D:34:ILE:CD1	4:D:61:ALA:HA	2.48	0.43
1:A:192:ILE:HG12	1:A:660:ILE:HD12	2.01	0.43
1:A:102:HIS:O	1:A:104:THR:N	2.50	0.43
1:A:366:GLY:O	1:A:442:ALA:HA	2.18	0.43
1:A:534:PHE:CE2	1:A:566:VAL:HG11	2.53	0.43
2:B:100:ILE:CD1	2:B:238:ILE:HD13	2.48	0.43
2:B:241:LEU:HD21	2:B:249:ILE:HD12	2.00	0.43
1:A:390:VAL:HG23	5:A:1705:NAG:H82	2.00	0.43
1:A:156:PHE:CD2	1:A:421:PRO:CD	2.99	0.43
3:C:62:ARG:HG2	3:C:68:GLN:CD	2.38	0.43
3:C:31:ARG:O	3:C:34:ILE:HG12	2.19	0.43
4:D:26:LEU:HB3	4:D:29:LEU:HB2	2.00	0.43
1:A:311:ALA:HB1	1:A:511:VAL:HG23	1.98	0.43
1:A:662:LEU:HD13	3:C:149:ILE:HA	2.01	0.43
1:A:68:GLY:N	1:A:218:PHE:HE1	2.12	0.43
1:A:367:GLN:O	1:A:443:ASP:CG	2.56	0.43
2:B:452:LEU:HD13	3:C:51:VAL:CG2	2.48	0.43
3:C:91:TYR:CE1	3:C:182:CYS:SG	3.11	0.43
1:A:224:VAL:CG2	4:D:100:THR:O	2.57	0.43
1:A:299:VAL:CG2	1:A:553:HIS:CD2	3.02	0.43
1:A:279:ALA:O	1:A:364:GLU:HA	2.18	0.43
2:B:432:LEU:N	2:B:433:PRO:HD3	2.34	0.43
1:A:112:LYS:HB3	1:A:112:LYS:HE2	1.82	0.42
1:A:97:LEU:HD13	1:A:192:ILE:CG2	2.49	0.42
3:C:112:ILE:HG13	3:C:117:MET:HG3	2.01	0.42
1:A:583:ARG:HA	1:A:604:TRP:NE1	2.35	0.42
1:A:605:VAL:HG13	1:A:619:ARG:O	2.19	0.42
1:A:306:LEU:HG	1:A:329:PHE:CE2	2.55	0.42
1:A:334:THR:HG23	1:A:335:PHE:CD2	2.55	0.42
1:A:385:GLN:C	1:A:391:ARG:HD3	2.40	0.42
1:A:157:ALA:C	1:A:158:HIS:ND1	2.73	0.42
1:A:356:LEU:HA	1:A:356:LEU:HD12	1.75	0.42
1:A:396:ASP:O	1:A:400:THR:HG23	2.19	0.42
1:A:341:SER:CB	1:A:429:ARG:HD2	2.49	0.42
2:B:465:PHE:HA	3:C:204:THR:HB	2.01	0.42
3:C:60:THR:HG21	3:C:67:LEU:CD2	2.45	0.42
1:A:312:LEU:HD11	1:A:498:LEU:CB	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:GLN:HG2	5:A:1710:NAG:H81	2.00	0.42
2:B:174:LEU:HD22	2:B:206:GLY:HA2	2.00	0.42
3:C:243:LEU:HD22	3:C:243:LEU:O	2.18	0.42
1:A:296:GLU:OE1	1:A:367:GLN:NE2	2.48	0.42
1:A:54:LEU:CD1	1:A:248:CYS:SG	3.06	0.42
1:A:378:MET:HE1	1:A:415:ARG:HE	1.84	0.42
1:A:74:HIS:O	1:A:96:VAL:HA	2.18	0.42
1:A:296:GLU:HG3	1:A:370:LEU:HD21	2.01	0.42
1:A:345:TYR:CE2	1:A:349:LYS:HE2	2.55	0.42
2:B:244:TRP:CE3	2:B:244:TRP:CA	3.03	0.42
3:C:17:ALA:CB	3:C:168:ILE:HG21	2.41	0.42
3:C:60:THR:O	3:C:61:ASP:HB3	2.20	0.42
2:B:186:PHE:CD1	2:B:193:VAL:HG21	2.55	0.42
4:D:38:PHE:CD1	4:D:38:PHE:C	2.92	0.42
1:A:279:ALA:HA	1:A:328:VAL:HG13	2.02	0.41
2:B:235:LEU:HD23	2:B:235:LEU:HA	1.91	0.41
2:B:247:TRP:CH2	2:B:395:LYS:HB3	2.53	0.41
3:C:34:ILE:CD1	3:C:120:VAL:CG1	2.98	0.41
3:C:163:LEU:HD21	3:C:204:THR:CG2	2.47	0.41
4:D:34:ILE:HD11	4:D:61:ALA:HA	2.01	0.41
4:D:45:PRO:HG2	4:D:46:ALA:N	2.34	0.41
1:A:234:SER:OG	1:A:246:ILE:HG23	2.19	0.41
2:B:195:TYR:CZ	4:D:94:PHE:HB2	2.55	0.41
1:A:158:HIS:O	1:A:159:CYS:SG	2.79	0.41
1:A:185:ASP:OD1	1:A:186:GLU:N	2.53	0.41
1:A:222:HIS:CB	1:A:247:VAL:HG23	2.50	0.41
1:A:279:ALA:HB1	1:A:330:PHE:CD2	2.53	0.41
1:A:162:ILE:HD11	1:A:421:PRO:HG2	2.03	0.41
1:A:429:ARG:NH2	1:A:432:ARG:NH1	2.68	0.41
2:B:433:PRO:HB3	2:B:436:PRO:HG3	2.02	0.41
1:A:162:ILE:HD12	1:A:164:TRP:CZ2	2.54	0.41
2:B:193:VAL:HG12	2:B:198:VAL:HG23	2.02	0.41
1:A:672:THR:HG23	3:C:158:LEU:HD13	2.03	0.41
1:A:453:TYR:CD2	1:A:454:GLN:HG2	2.55	0.41
1:A:553:HIS:HD1	1:A:563:THR:HG21	1.85	0.41
1:A:68:GLY:CA	1:A:218:PHE:HD1	2.30	0.41
3:C:115:ARG:NH1	7:C:1245:PC1:O12	2.48	0.41
1:A:375:GLU:HA	1:A:412:ILE:HG23	2.02	0.41
1:A:451:LYS:CB	1:A:451:LYS:NZ	2.73	0.41
1:A:258:SER:HB2	1:A:571:LEU:HD21	2.03	0.41
1:A:159:CYS:O	1:A:159:CYS:SG	2.79	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:251:ALA:O	2:B:255:VAL:HG23	2.21	0.41
3:C:91:TYR:CZ	3:C:182:CYS:SG	3.13	0.41
4:D:82:ARG:NH2	4:D:97:PRO:HG3	2.35	0.41
2:B:246:ALA:HB1	2:B:395:LYS:HG3	2.02	0.41
1:A:234:SER:HB2	1:A:247:VAL:HG12	2.02	0.41
1:A:352:PHE:CD1	1:A:353:PRO:HD2	2.56	0.41
1:A:57:THR:CG2	1:A:58:HIS:ND1	2.83	0.41
1:A:672:THR:HG23	3:C:158:LEU:CD1	2.50	0.41
1:A:101:LYS:HG2	1:A:126:THR:HG21	2.02	0.41
1:A:167:LEU:HD22	1:A:451:LYS:HG2	2.02	0.41
1:A:215:MET:HE2	1:A:215:MET:HB3	1.79	0.41
1:A:304:THR:HG22	1:A:487:LEU:CG	2.51	0.41
1:A:361:SER:CB	1:A:501:LEU:HD13	2.48	0.41
1:A:64:SER:HB3	1:A:219:SER:O	2.20	0.41
1:A:256:VAL:HG21	1:A:567:VAL:CG1	2.48	0.40
1:A:349:LYS:HB3	1:A:351:LYS:CD	2.50	0.40
1:A:52:ARG:HG2	1:A:54:LEU:HD21	2.03	0.40
1:A:125:LEU:HD12	1:A:125:LEU:HA	1.85	0.40
1:A:140:CYS:CB	1:A:159:CYS:HG	2.33	0.40
2:B:241:LEU:HD12	2:B:241:LEU:HA	1.76	0.40
1:A:328:VAL:HG22	1:A:329:PHE:N	2.36	0.40
1:A:460:ALA:HB1	1:A:465:VAL:HB	2.03	0.40
2:B:248:LEU:HD22	2:B:252:VAL:HG23	2.03	0.40
2:B:192:ALA:HB3	4:D:79:GLN:HE22	1.86	0.40
1:A:169:ASN:HD22	1:A:171:LEU:HB2	1.85	0.40
1:A:332:GLY:HA2	1:A:555:ILE:HG12	2.03	0.40
1:A:378:MET:HA	1:A:440:VAL:O	2.21	0.40
1:A:53:LEU:HB2	1:A:60:ILE:HD11	2.02	0.40
1:A:60:ILE:HG12	1:A:648:TRP:HZ3	1.85	0.40
3:C:35:LEU:HA	3:C:124:SER:HB2	2.03	0.40
1:A:380:THR:O	1:A:382:PRO:HD3	2.21	0.40
1:A:283:ASP:CG	1:A:555:ILE:HD11	2.42	0.40
1:A:60:ILE:O	1:A:60:ILE:HG13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	663/709 (94%)	589 (89%)	54 (8%)	20 (3%)	5	35
2	B	209/467 (45%)	196 (94%)	8 (4%)	5 (2%)	7	40
3	C	241/265 (91%)	228 (95%)	12 (5%)	1 (0%)	38	75
4	D	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
All	All	1211/1542 (78%)	1108 (92%)	77 (6%)	26 (2%)	12	43

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	472	SER
1	A	559	SER
1	A	210	PHE
1	A	333	GLU
1	A	371	ARG
1	A	435	ASN
1	A	454	GLN
1	A	473	PRO
2	B	216	LYS
2	B	403	ASP
1	A	211	PRO
1	A	612	ASN
2	B	105	PHE
1	A	88	ASP
1	A	560	PRO
1	A	163	GLN
1	A	223	ALA
1	A	353	PRO
2	B	435	LEU
3	C	107	ASP
1	A	89	GLY
1	A	646	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	655	ASP
1	A	480	VAL
2	B	432	LEU
1	A	129	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	583/612 (95%)	497 (85%)	86 (15%)	3	19
2	B	184/408 (45%)	165 (90%)	19 (10%)	8	35
3	C	193/214 (90%)	171 (89%)	22 (11%)	7	29
4	D	88/89 (99%)	77 (88%)	11 (12%)	5	25
All	All	1048/1323 (79%)	910 (87%)	138 (13%)	8	23

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	59	GLN
1	A	60	ILE
1	A	69	ASP
1	A	84	TRP
1	A	85	VAL
1	A	86	LEU
1	A	94	TYR
1	A	95	MET
1	A	97	LEU
1	A	101	LYS
1	A	104	THR
1	A	107	LEU
1	A	111	LEU
1	A	112	LYS
1	A	121	LEU
1	A	126	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	129	SER
1	A	132	SER
1	A	139	GLN
1	A	147	VAL
1	A	149	SER
1	A	150	ASN
1	A	152	TYR
1	A	155	GLU
1	A	162	ILE
1	A	163	GLN
1	A	174	GLU
1	A	182	LEU
1	A	201	LEU
1	A	210	PHE
1	A	217	LEU
1	A	248	CYS
1	A	249	ASP
1	A	264	ASN
1	A	270	LYS
1	A	273	ASP
1	A	280	THR
1	A	281	ARG
1	A	296	GLU
1	A	302	PHE
1	A	305	GLN
1	A	306	LEU
1	A	312	LEU
1	A	326	MET
1	A	333	GLU
1	A	342	ARG
1	A	343	MET
1	A	347	MET
1	A	349	LYS
1	A	364	GLU
1	A	365	LEU
1	A	367	GLN
1	A	371	ARG
1	A	378	MET
1	A	380	THR
1	A	387	ASN
1	A	391	ARG
1	A	413	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	418	GLN
1	A	425	SER
1	A	429	ARG
1	A	431	LEU
1	A	434	ARG
1	A	436	ILE
1	A	437	SER
1	A	463	ILE
1	A	464	ASN
1	A	487	LEU
1	A	537	ILE
1	A	561	THR
1	A	562	ASN
1	A	574	LEU
1	A	586	CYS
1	A	604	TRP
1	A	605	VAL
1	A	609	LEU
1	A	624	THR
1	A	631	LEU
1	A	632	SER
1	A	636	GLU
1	A	637	LEU
1	A	638	SER
1	A	643	THR
1	A	644	GLU
1	A	695	ASP
2	B	84	MET
2	B	85	LEU
2	B	91	LEU
2	B	174	LEU
2	B	180	ILE
2	B	241	LEU
2	B	244	TRP
2	B	248	LEU
2	B	381	LEU
2	B	395	LYS
2	B	407	THR
2	B	420	LEU
2	B	422	LEU
2	B	423	LEU
2	B	424	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	425	LEU
2	B	427	ILE
2	B	429	LYS
2	B	435	LEU
3	C	46	LEU
3	C	47	LEU
3	C	64	ASP
3	C	68	GLN
3	C	91	TYR
3	C	93	LEU
3	C	106	GLU
3	C	112	ILE
3	C	113	SER
3	C	114	ILE
3	C	123	LEU
3	C	127	ILE
3	C	133	SER
3	C	146	VAL
3	C	170	LEU
3	C	192	LEU
3	C	206	LEU
3	C	207	ASN
3	C	218	TYR
3	C	242	SER
3	C	243	LEU
3	C	244	LEU
4	D	14	LEU
4	D	38	PHE
4	D	39	ARG
4	D	40	GLU
4	D	42	PHE
4	D	43	LEU
4	D	47	TYR
4	D	50	GLN
4	D	67	TRP
4	D	94	PHE
4	D	98	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	150	ASN
1	A	163	GLN
1	A	169	ASN
1	A	222	HIS
1	A	305	GLN
1	A	313	GLN
1	A	331	GLN
1	A	358	ASN
1	A	393	GLN
1	A	418	GLN
1	A	428	GLN
1	A	478	ASN
1	A	516	GLN
1	A	531	ASN
1	A	606	GLN
1	A	639	GLN
3	C	116	GLN
3	C	136	ASN
3	C	207	ASN
4	D	8	ASN
4	D	79	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

22 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	A	1699	1,5	14,14,15	0.57	0	15,19,21	1.10	1 (6%)
5	NAG	A	1700	5	14,14,15	0.50	0	15,19,21	1.35	3 (20%)
5	NAG	A	1701	1,5	14,14,15	0.49	0	15,19,21	1.56	2 (13%)
5	NAG	A	1702	5,6	14,14,15	0.48	0	15,19,21	0.93	0
5	NAG	A	1703	1,5	14,14,15	0.62	0	15,19,21	1.41	1 (6%)
5	NAG	A	1704	5	14,14,15	0.56	0	15,19,21	1.44	4 (26%)
5	NAG	A	1705	1	14,14,15	0.54	0	15,19,21	1.09	1 (6%)
5	NAG	A	1706	1,5	14,14,15	0.49	0	15,19,21	1.21	2 (13%)
5	NAG	A	1707	5	14,14,15	0.53	0	15,19,21	1.25	3 (20%)
5	NAG	A	1708	1,5	14,14,15	0.51	0	15,19,21	1.21	2 (13%)
5	NAG	A	1709	5	14,14,15	0.72	0	15,19,21	2.35	6 (40%)
5	NAG	A	1710	1,5	14,14,15	0.66	0	15,19,21	1.04	1 (6%)
5	NAG	A	1711	5	14,14,15	0.47	0	15,19,21	0.75	0
5	NAG	A	1712	1	14,14,15	0.44	0	15,19,21	1.10	1 (6%)
5	NAG	A	1713	1	14,14,15	0.52	0	15,19,21	1.24	1 (6%)
5	NAG	A	1714	1	14,14,15	0.48	0	15,19,21	0.80	0
5	NAG	A	1715	1	14,14,15	0.47	0	15,19,21	0.94	1 (6%)
6	BMA	A	1716	5,6	11,11,12	0.39	0	13,15,17	0.95	1 (7%)
6	BMA	A	1717	6	11,11,12	0.40	0	13,15,17	1.56	2 (15%)
6	BMA	A	1718	6	11,11,12	0.32	0	13,15,17	0.66	0
7	PC1	B	1468	-	42,42,53	1.04	2 (4%)	47,50,61	1.05	2 (4%)
7	PC1	C	1245	-	42,42,53	1.06	2 (4%)	47,50,61	1.01	3 (6%)

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	A	1699	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1700	5	-	0/6/23/26	0/1/1/1
5	NAG	A	1701	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1702	5,6	-	0/6/23/26	0/1/1/1
5	NAG	A	1703	1,5	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1704	5	-	0/6/23/26	0/1/1/1
5	NAG	A	1705	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1706	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1707	5	-	0/6/23/26	0/1/1/1
5	NAG	A	1708	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1709	5	-	0/6/23/26	0/1/1/1
5	NAG	A	1710	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1711	5	-	0/6/23/26	0/1/1/1
5	NAG	A	1712	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1713	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1714	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1715	1	-	0/6/23/26	0/1/1/1
6	BMA	A	1716	5,6	-	0/2/19/22	0/1/1/1
6	BMA	A	1717	6	-	0/2/19/22	0/1/1/1
6	BMA	A	1718	6	-	0/2/19/22	0/1/1/1
7	PC1	B	1468	-	-	0/46/46/57	0/0/0/0
7	PC1	C	1245	-	-	0/46/46/57	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1468	PC1	O21-C21	4.17	1.46	1.34
7	C	1245	PC1	O21-C21	4.27	1.46	1.34
7	B	1468	PC1	O31-C31	4.30	1.46	1.33
7	C	1245	PC1	O31-C31	4.40	1.46	1.33

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1713	NAG	O5-C1-C2	-3.37	106.78	111.47
5	A	1712	NAG	O5-C1-C2	-3.22	107.00	111.47
5	A	1709	NAG	O7-C7-C8	-2.82	116.93	122.06
5	A	1705	NAG	O5-C1-C2	-2.67	107.75	111.47
5	A	1708	NAG	O5-C1-C2	-2.40	108.13	111.47
5	A	1704	NAG	O5-C1-C2	-2.39	108.14	111.47
5	A	1715	NAG	O5-C1-C2	-2.22	108.38	111.47
5	A	1709	NAG	O5-C1-C2	-2.22	108.39	111.47
5	A	1706	NAG	C4-C3-C2	-2.13	107.90	111.02
7	C	1245	PC1	O31-C31-O32	-2.10	118.34	123.55
5	A	1700	NAG	O5-C1-C2	-2.06	108.61	111.47
5	A	1710	NAG	C3-C4-C5	-2.02	106.67	110.22
5	A	1701	NAG	C8-C7-N2	2.06	119.83	116.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1707	NAG	C2-N2-C7	2.08	125.98	122.94
6	A	1716	BMA	C3-C4-C5	2.16	114.02	110.22
5	A	1707	NAG	C1-O5-C5	2.17	115.16	112.17
5	A	1704	NAG	C4-C3-C2	2.19	114.23	111.02
5	A	1706	NAG	O4-C4-C5	2.20	114.83	109.28
5	A	1704	NAG	C3-C4-C5	2.21	114.11	110.22
5	A	1700	NAG	C2-N2-C7	2.33	126.34	122.94
5	A	1708	NAG	C4-C3-C2	2.36	114.48	111.02
5	A	1707	NAG	C8-C7-N2	2.39	120.42	116.11
5	A	1704	NAG	C8-C7-N2	2.43	120.50	116.11
6	A	1717	BMA	C3-C4-C5	2.64	114.87	110.22
5	A	1700	NAG	C8-C7-N2	2.69	120.97	116.11
7	B	1468	PC1	O31-C31-C32	2.74	119.87	111.90
5	A	1699	NAG	C4-C3-C2	2.79	115.11	111.02
7	C	1245	PC1	O31-C31-C32	2.89	120.30	111.90
5	A	1709	NAG	C3-C4-C5	3.64	116.62	110.22
5	A	1709	NAG	C8-C7-N2	3.83	123.03	116.11
5	A	1709	NAG	C4-C3-C2	4.07	116.98	111.02
7	C	1245	PC1	O21-C21-C22	4.11	120.08	111.55
7	B	1468	PC1	O21-C21-C22	4.20	120.27	111.55
5	A	1703	NAG	C1-O5-C5	4.43	118.27	112.17
5	A	1709	NAG	C2-N2-C7	4.48	129.48	122.94
5	A	1701	NAG	C1-O5-C5	4.51	118.39	112.17
6	A	1717	BMA	C1-O5-C5	4.62	118.53	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1705	NAG	2	0
5	A	1706	NAG	1	0
5	A	1707	NAG	1	0
5	A	1710	NAG	2	0
5	A	1714	NAG	1	0
7	C	1245	PC1	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.