



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 7, 2017 – 01:01 PM EST

PDB ID : 5H7I
EMDB ID: : EMD-6671
Title : Cryo-EM structure of the Cdt1-MCM2-7 complex in AMPPNP state
Authors : Zhai, Y.; Cheng, E.; Wu, H.; Li, N.; Yung, P.Y.; Gao, N.; Tye, B.K.
Deposited on : 2016-11-18
Resolution : 7.10 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 : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

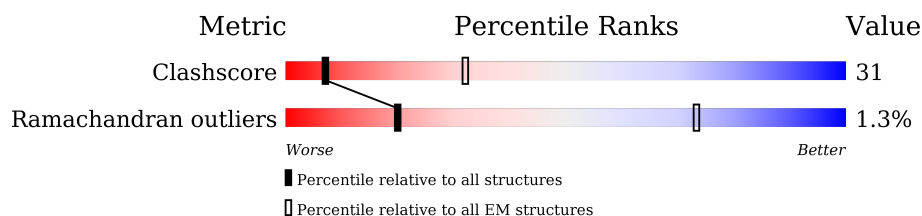
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.10 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	114402	924
Ramachandran outliers	111179	726

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	2	868	47% 20% . 32%
2	3	971	44% 18% . 38%
3	4	933	52% 24% . 23%
4	5	775	62% 19% 18%
5	6	1017	38% 23% . 36%
6	7	845	51% 22% 26%
7	C	604	51% 18% . 29%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 21016 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 DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	2	591	Total	C	N	O	0	0
			2924	1742	591	591		

- Molecule 2 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	3	601	Total	C	N	O	0	0
			2974	1772	601	601		

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	4	716	Total	C	N	O	0	0
			3551	2119	716	716		

- Molecule 4 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	5	632	Total	C	N	O	0	0
			3130	1866	632	632		

- Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	6	652	Total	C	N	O	0	0
			3230	1926	652	652		

- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	7	622	Total	C	N	O	0	0
			3076	1832	622	622		

- Molecule 7 is a protein called Cell division cycle protein CDT1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	C	429	2131	1273	429	429	0	0

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	63000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 2$	RMSZ	# $ Z > 2$
1	2	0.52	0/2920	0.69	3/4063 (0.1%)
2	3	0.45	0/2968	0.62	0/4127
3	4	0.51	0/3546	0.69	4/4939 (0.1%)
4	5	0.39	0/3121	0.56	0/4337
5	6	0.54	0/3221	0.77	5/4477 (0.1%)
6	7	0.46	0/3071	0.64	0/4271
7	C	0.42	0/2126	0.71	2/2960 (0.1%)
All	All	0.48	0/20973	0.67	14/29174 (0.0%)

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	2	0	6
2	3	0	5
3	4	0	6
4	5	0	2
5	6	0	19
6	7	0	6
7	C	0	17
All	All	0	61

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	6	626	GLY	N-CA-C	-6.63	96.52	113.10
5	6	561	GLU	N-CA-C	-6.51	93.41	111.00
1	2	334	LEU	N-CA-C	-6.49	93.48	111.00
1	2	570	GLY	N-CA-C	6.27	128.77	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4	920	GLY	C-N-CA	-5.95	106.81	121.70
5	6	767	LYS	N-CA-C	5.84	126.78	111.00
5	6	624	GLU	C-N-CA	-5.57	107.78	121.70
5	6	720	ASN	N-CA-C	-5.53	96.06	111.00
1	2	366	ASN	C-N-CA	5.29	134.93	121.70
3	4	919	LEU	N-CA-C	5.22	125.10	111.00
3	4	376	CYS	C-N-CA	5.21	134.73	121.70
3	4	376	CYS	CA-C-N	5.18	128.60	117.20
7	C	220	VAL	N-CA-C	5.11	124.80	111.00
7	C	199	PHE	C-N-CA	-5.11	100.54	122.00

There are no chirality outliers.

All (61) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	218	TYR	Peptide
1	2	298	SER	Peptide
1	2	367	CYS	Peptide
1	2	434	TYR	Peptide
1	2	588	GLU	Peptide
1	2	803	PHE	Peptide
2	3	172	THR	Peptide
2	3	237	GLU	Peptide
2	3	300	SER	Peptide
2	3	428	LEU	Peptide
2	3	498	ALA	Peptide
3	4	179	ILE	Peptide
3	4	373	ARG	Peptide
3	4	393	ASP	Peptide
3	4	408	ASP	Peptide
3	4	714	GLU	Peptide
3	4	927	VAL	Peptide
4	5	170	SER	Peptide
4	5	460	ARG	Mainchain
5	6	133	GLU	Peptide
5	6	321	VAL	Peptide
5	6	339	GLU	Peptide
5	6	354	LEU	Peptide
5	6	355	ASP	Peptide
5	6	356	TRP	Peptide
5	6	400	VAL	Peptide
5	6	402	ILE	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
5	6	559	THR	Peptide
5	6	561	GLU	Peptide
5	6	578	SER	Peptide
5	6	581	LYS	Peptide
5	6	605	ALA	Peptide
5	6	627	ALA	Peptide
5	6	662	SER	Peptide
5	6	700	ASN	Peptide
5	6	764	ILE	Peptide
5	6	780	LEU	Peptide
5	6	972	ASP	Peptide
6	7	209	GLN	Peptide
6	7	371	LEU	Peptide
6	7	504	ASP	Peptide
6	7	678	LYS	Peptide
6	7	680	SER	Peptide
6	7	94	LEU	Peptide
7	C	146	SER	Peptide
7	C	196	LEU	Peptide
7	C	203	LYS	Peptide
7	C	210	SER	Peptide
7	C	215	THR	Peptide
7	C	219	TRP	Peptide
7	C	220	VAL	Peptide
7	C	226	ASP	Peptide
7	C	307	LEU	Peptide
7	C	334	THR	Peptide
7	C	386	PRO	Peptide
7	C	47	ASN	Peptide
7	C	599	LYS	Peptide
7	C	63	THR	Peptide
7	C	64	LYS	Peptide
7	C	77	PHE	Peptide
7	C	83	LEU	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	2	2924	0	1308	149	0
2	3	2974	0	1349	134	0
3	4	3551	0	1537	162	0
4	5	3130	0	1369	97	0
5	6	3230	0	1449	202	0
6	7	3076	0	1381	157	0
7	C	2131	0	919	78	0
All	All	21016	0	9312	939	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

All (939) 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)
1:2:386:GLN:N	1:2:410:LEU:O	1.57	1.36
3:4:856:VAL:HA	3:4:860:LYS:CB	1.73	1.19
5:6:625:ALA:HB3	5:6:629:MET:H	1.04	1.13
2:3:190:SER:HA	2:3:456:ARG:HA	1.34	1.09
1:2:386:GLN:O	1:2:410:LEU:N	1.86	1.08
5:6:512:GLU:O	5:6:515:GLU:N	1.86	1.08
3:4:855:SER:HA	3:4:860:LYS:CB	1.81	1.06
5:6:608:LEU:HA	5:6:625:ALA:HA	1.37	1.05
6:7:250:ASP:N	6:7:505:GLU:O	1.89	1.04
2:3:197:ILE:O	2:3:198:ARG:O	1.75	1.02
6:7:249:SER:HA	6:7:507:ILE:HA	1.38	1.01
7:C:208:LYS:N	7:C:248:PRO:O	1.96	0.97
3:4:854:LYS:O	3:4:857:ILE:N	1.98	0.96
3:4:655:SER:HA	3:4:664:THR:HA	1.47	0.95
3:4:352:CYS:N	3:4:373:ARG:O	2.00	0.95
6:7:618:TYR:O	6:7:622:HIS:N	2.00	0.94
5:6:777:TYR:O	5:6:781:ARG:CB	2.17	0.93
3:4:856:VAL:CA	3:4:860:LYS:CB	2.46	0.92
1:2:355:SER:O	1:2:434:TYR:N	2.02	0.92
1:2:630:SER:HA	1:2:639:THR:HA	1.51	0.92
5:6:405:PRO:HA	5:6:450:TYR:HA	1.51	0.89
2:3:434:GLY:N	2:3:473:ASP:O	2.05	0.89
1:2:526:ASN:HA	1:2:532:SER:HA	1.55	0.89
1:2:242:LEU:O	1:2:296:ARG:N	2.06	0.88
5:6:625:ALA:HB3	5:6:629:MET:N	1.87	0.88
6:7:254:ALA:N	6:7:308:SER:O	2.05	0.88
2:3:188:LYS:HA	2:3:458:GLU:HA	1.55	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:205:ILE:O	7:C:222:ILE:N	2.06	0.88
7:C:573:GLN:HA	7:C:578:LEU:HA	1.56	0.88
3:4:855:SER:CA	3:4:860:LYS:CB	2.46	0.87
1:2:341:CYS:HA	1:2:373:PHE:HA	1.55	0.87
3:4:550:LYS:O	3:4:557:ARG:N	2.07	0.87
5:6:525:ILE:O	5:6:529:LEU:N	2.07	0.87
6:7:334:HIS:HA	6:7:503:THR:N	1.89	0.87
5:6:159:SER:HA	5:6:167:ALA:HB2	1.57	0.86
5:6:503:VAL:O	5:6:506:ASN:N	2.09	0.85
1:2:425:GLU:O	1:2:457:LYS:N	2.09	0.85
5:6:404:VAL:O	5:6:451:LYS:N	2.10	0.85
3:4:441:SER:HA	3:4:459:THR:HA	1.58	0.84
3:4:733:PRO:CB	6:7:445:GLY:H	1.91	0.84
5:6:527:ASP:O	5:6:531:ARG:N	2.10	0.83
6:7:543:GLN:O	6:7:545:THR:N	2.11	0.83
1:2:386:GLN:C	1:2:410:LEU:H	1.80	0.83
3:4:378:GLU:O	3:4:380:ASN:N	2.11	0.83
1:2:560:ALA:HB3	1:2:563:ALA:HB2	1.60	0.82
2:3:504:THR:HA	6:7:326:HIS:HA	1.60	0.82
2:3:452:THR:HA	6:7:368:ALA:H	1.45	0.82
1:2:327:ARG:C	1:2:590:THR:HA	1.99	0.82
3:4:855:SER:H	3:4:859:ARG:CB	1.93	0.82
5:6:143:MET:O	5:6:147:ASP:N	2.11	0.82
2:3:449:ASP:HA	2:3:455:ARG:HA	1.62	0.81
3:4:608:ASP:N	3:4:613:GLN:O	2.12	0.81
5:6:151:ILE:N	5:6:264:GLN:O	2.13	0.81
5:6:578:SER:HA	5:6:581:LYS:N	1.96	0.81
6:7:80:ILE:N	6:7:203:TYR:O	2.13	0.81
1:2:548:ALA:O	1:2:551:GLN:N	2.14	0.81
2:3:190:SER:CA	2:3:456:ARG:HA	2.09	0.81
3:4:607:ARG:HA	3:4:614:LEU:HA	1.61	0.81
4:5:734:ARG:O	4:5:738:VAL:CB	2.29	0.81
5:6:578:SER:HA	5:6:581:LYS:H	1.45	0.81
7:C:207:TYR:HA	7:C:249:LEU:HA	1.59	0.81
3:4:343:LYS:O	3:4:360:ILE:N	2.12	0.80
5:6:779:GLU:O	5:6:783:ASP:CB	2.29	0.80
5:6:303:GLU:O	5:6:353:PHE:HA	1.80	0.80
5:6:794:ARG:H	5:6:795:ILE:HA	1.46	0.80
5:6:797:VAL:O	5:6:800:LEU:N	2.13	0.80
5:6:506:ASN:O	5:6:510:SER:N	2.12	0.80
5:6:314:CYS:N	5:6:336:PRO:O	2.14	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:224:ARG:H	7:C:83:LEU:HA	1.46	0.80
5:6:123:SER:N	5:6:134:LYS:O	2.14	0.80
1:2:326:ARG:HA	1:2:591:LEU:C	2.01	0.80
5:6:608:LEU:CA	5:6:625:ALA:HA	2.11	0.80
5:6:288:LEU:O	5:6:399:GLY:N	2.15	0.79
5:6:596:VAL:O	5:6:637:CYS:N	2.14	0.79
5:6:720:ASN:O	5:6:724:ASP:N	2.15	0.79
3:4:485:LEU:N	7:C:575:ASP:O	2.15	0.79
5:6:406:ASP:N	5:6:449:THR:O	2.13	0.79
7:C:206:ARG:H	7:C:250:GLN:C	1.85	0.79
1:2:540:LEU:N	1:2:679:ILE:O	2.14	0.79
5:6:403:VAL:HA	5:6:452:ILE:HA	1.64	0.78
2:3:734:ARG:O	2:3:738:LEU:N	2.13	0.78
7:C:205:ILE:HA	7:C:251:ILE:HA	1.64	0.78
1:2:328:THR:CB	1:2:387:ARG:CB	2.61	0.78
2:3:537:ASP:O	2:3:540:LEU:N	2.16	0.77
4:5:171:VAL:N	4:5:254:GLN:O	2.16	0.77
3:4:399:LEU:O	3:4:415:ILE:N	2.15	0.77
6:7:255:VAL:HA	6:7:307:PHE:HA	1.66	0.77
2:3:30:GLU:O	2:3:34:THR:N	2.12	0.77
6:7:247:ARG:H	6:7:509:GLU:HA	1.49	0.77
3:4:856:VAL:C	3:4:860:LYS:CB	2.54	0.76
2:3:186:VAL:O	2:3:289:GLY:N	2.16	0.76
2:3:442:LEU:H	2:3:460:GLY:HA3	1.50	0.76
2:3:254:GLN:HA	2:3:454:GLU:CB	2.15	0.76
1:2:334:LEU:O	1:2:381:VAL:CB	2.33	0.76
6:7:225:LEU:H	6:7:241:VAL:HA	1.51	0.76
7:C:372:VAL:O	7:C:384:ASN:N	2.16	0.76
5:6:635:ILE:HA	5:6:677:SER:O	1.86	0.76
6:7:350:ASP:N	6:7:382:ARG:O	2.16	0.76
5:6:661:ILE:N	5:6:672:LEU:O	2.19	0.75
6:7:249:SER:HA	6:7:507:ILE:CA	2.15	0.75
1:2:497:ILE:O	1:2:500:SER:N	2.19	0.75
1:2:328:THR:N	1:2:387:ARG:O	2.16	0.75
3:4:605:ILE:HA	3:4:616:LEU:HA	1.68	0.75
6:7:311:GLN:HA	6:7:504:ASP:O	1.86	0.75
2:3:188:LYS:O	2:3:457:LEU:N	2.19	0.75
2:3:295:VAL:O	2:3:324:ASN:N	2.20	0.75
5:6:516:LEU:O	5:6:519:MET:N	2.20	0.74
2:3:408:VAL:N	2:3:547:PHE:O	2.19	0.74
5:6:598:THR:N	5:6:637:CYS:O	2.16	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:446:VAL:N	2:3:456:ARG:O	2.20	0.74
5:6:303:GLU:H	5:6:354:LEU:H	1.32	0.74
5:6:572:CYS:O	5:6:712:PHE:HA	1.86	0.74
2:3:191:LEU:N	2:3:455:ARG:O	2.20	0.74
3:4:733:PRO:C	6:7:445:GLY:HA2	2.07	0.73
2:3:496:THR:HA	2:3:505:THR:HA	1.70	0.73
3:4:573:SER:O	3:4:576:GLN:N	2.21	0.73
1:2:327:ARG:H	1:2:591:LEU:N	1.86	0.73
1:2:547:THR:C	1:2:549:LYS:H	1.90	0.73
7:C:527:GLN:O	7:C:529:TYR:N	2.20	0.73
3:4:853:GLY:C	3:4:858:GLN:H	1.91	0.73
5:6:303:GLU:N	5:6:354:LEU:H	1.86	0.73
5:6:581:LYS:CB	5:6:583:GLN:H	2.02	0.73
4:5:496:ALA:O	4:5:500:GLN:N	2.22	0.73
4:5:530:TYR:O	4:5:534:LYS:N	2.16	0.73
2:3:452:THR:HA	6:7:368:ALA:N	2.04	0.72
3:4:654:ILE:O	3:4:665:LEU:N	2.22	0.72
5:6:633:ASN:N	5:6:675:ARG:O	2.19	0.72
5:6:648:ASP:O	5:6:651:ALA:N	2.22	0.72
6:7:334:HIS:N	6:7:376:LEU:O	2.21	0.72
3:4:248:LEU:O	3:4:251:TYR:N	2.23	0.72
1:2:623:ALA:O	1:2:627:GLN:N	2.17	0.72
6:7:80:ILE:O	6:7:205:LYS:N	2.22	0.72
1:2:315:SER:N	1:2:430:TYR:O	2.17	0.72
2:3:190:SER:HA	2:3:456:ARG:CA	2.16	0.72
1:2:337:VAL:N	1:2:351:PHE:O	2.22	0.72
1:2:525:LYS:N	1:2:532:SER:O	2.23	0.72
1:2:331:PHE:O	1:2:384:ASN:N	2.23	0.71
4:5:171:VAL:CB	4:5:460:ARG:O	2.37	0.71
7:C:351:MET:C	7:C:353:ARG:H	1.90	0.71
6:7:254:ALA:O	6:7:308:SER:N	2.23	0.71
5:6:117:GLN:O	5:6:121:ASP:N	2.23	0.71
2:3:194:PRO:HA	2:3:252:ASP:HA	1.72	0.71
3:4:831:SER:O	3:4:835:ASP:N	2.23	0.71
2:3:61:ASP:HA	6:7:212:ALA:C	2.11	0.71
1:2:386:GLN:O	1:2:409:ILE:HA	1.90	0.71
2:3:461:ALA:O	2:3:465:ALA:N	2.24	0.71
4:5:452:SER:O	4:5:465:GLU:N	2.23	0.70
4:5:503:SER:HA	4:5:512:VAL:HA	1.74	0.70
5:6:608:LEU:H	5:6:626:GLY:H	1.39	0.70
1:2:695:LEU:O	1:2:698:PHE:N	2.25	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:690:ASP:O	2:3:694:LYS:N	2.25	0.70
3:4:918:VAL:CB	3:4:926:SER:O	2.38	0.70
6:7:650:PRO:HA	6:7:706:ASP:HA	1.73	0.70
2:3:443:THR:HA	2:3:458:GLU:O	1.91	0.70
3:4:202:LYS:HA	3:4:224:LEU:HA	1.73	0.70
5:6:396:LYS:N	5:6:460:ILE:O	2.24	0.70
2:3:191:LEU:H	2:3:455:ARG:N	1.90	0.70
5:6:664:ALA:HA	5:6:668:ILE:O	1.92	0.69
4:5:182:MET:O	4:5:242:ILE:N	2.22	0.69
4:5:183:CYS:N	4:5:188:HIS:O	2.23	0.69
6:7:249:SER:N	6:7:312:GLU:O	2.24	0.69
6:7:499:LYS:HA	6:7:506:MET:H	1.57	0.69
3:4:345:ALA:O	3:4:357:ALA:HB1	1.92	0.69
3:4:399:LEU:N	3:4:415:ILE:O	2.14	0.69
5:6:607:GLY:CA	5:6:627:ALA:H	2.04	0.69
7:C:206:ARG:N	7:C:250:GLN:O	2.26	0.69
4:5:505:ALA:HA	4:5:510:THR:HA	1.74	0.69
1:2:223:GLY:HA2	7:C:86:ASP:H	1.58	0.69
3:4:188:GLN:O	3:4:190:CYS:N	2.23	0.69
7:C:206:ARG:O	7:C:250:GLN:N	2.26	0.68
1:2:629:ILE:O	1:2:640:LEU:N	2.27	0.68
1:2:328:THR:HA	1:2:589:TRP:C	2.13	0.68
4:5:729:SER:O	4:5:732:THR:N	2.24	0.68
6:7:334:HIS:HA	6:7:503:THR:H	1.59	0.68
3:4:377:ASN:CB	3:4:378:GLU:HA	2.24	0.68
4:5:173:SER:O	4:5:252:ASP:HA	1.94	0.68
4:5:300:ILE:HA	4:5:326:PRO:HA	1.73	0.68
6:7:25:LEU:O	6:7:27:THR:N	2.25	0.68
5:6:608:LEU:H	5:6:626:GLY:N	1.92	0.67
2:3:103:LEU:O	2:3:107:ASP:N	2.27	0.67
5:6:603:SER:H	5:6:604:SER:HA	1.59	0.67
5:6:634:GLY:O	5:6:677:SER:N	2.28	0.67
6:7:357:PRO:HA	6:7:374:THR:HA	1.75	0.67
5:6:720:ASN:O	5:6:723:ILE:N	2.28	0.67
1:2:224:ARG:H	7:C:83:LEU:CA	2.06	0.67
1:2:386:GLN:CA	1:2:410:LEU:O	2.43	0.67
2:3:391:LYS:O	2:3:399:LEU:N	2.26	0.67
3:4:348:LYS:O	3:4:383:SER:N	2.28	0.67
3:4:601:LEU:HA	3:4:620:ALA:HB3	1.76	0.67
3:4:734:GLU:N	6:7:445:GLY:HA2	2.10	0.67
1:2:326:ARG:HA	1:2:591:LEU:O	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:153:ILE:N	5:6:266:SER:O	2.24	0.67
2:3:61:ASP:O	6:7:213:ARG:HA	1.93	0.67
2:3:211:TYR:N	6:7:6:PRO:O	2.28	0.67
3:4:604:TYR:N	3:4:617:GLU:O	2.25	0.66
1:2:776:PRO:HA	1:2:827:GLU:C	2.16	0.66
5:6:524:HIS:O	5:6:527:ASP:N	2.27	0.66
6:7:25:LEU:C	6:7:27:THR:H	1.96	0.66
5:6:335:ASN:H	5:6:339:GLU:HA	1.60	0.66
7:C:206:ARG:HA	7:C:221:SER:N	2.10	0.66
2:3:98:ILE:O	2:3:158:LYS:N	2.27	0.66
7:C:36:ILE:O	7:C:41:ASP:N	2.28	0.66
2:3:194:PRO:O	6:7:372:THR:N	2.28	0.66
7:C:35:ALA:O	7:C:39:GLN:N	2.29	0.66
6:7:260:TYR:O	6:7:269:VAL:N	2.28	0.65
6:7:350:ASP:O	6:7:382:ARG:N	2.26	0.65
6:7:617:THR:O	6:7:621:MET:CB	2.44	0.65
1:2:354:ASP:O	1:2:356:ASN:HA	1.97	0.65
5:6:660:THR:HA	5:6:673:ASN:HA	1.77	0.65
6:7:89:GLN:O	6:7:93:PHE:N	2.30	0.65
1:2:542:LEU:N	1:2:681:CYS:O	2.29	0.65
4:5:502:ILE:O	4:5:513:LEU:N	2.30	0.65
1:2:777:LYS:H	1:2:828:PHE:HA	1.60	0.65
3:4:456:LEU:HA	6:7:253:PRO:O	1.97	0.65
2:3:495:VAL:O	2:3:506:LEU:N	2.28	0.65
3:4:918:VAL:CB	3:4:925:ARG:O	2.44	0.65
5:6:335:ASN:N	5:6:339:GLU:HA	2.12	0.65
4:5:176:ALA:O	4:5:178:TYR:N	2.30	0.64
6:7:68:GLN:O	6:7:72:ASN:N	2.26	0.64
4:5:770:ILE:O	4:5:774:GLY:N	2.31	0.64
5:6:103:VAL:O	5:6:107:THR:N	2.23	0.64
6:7:446:ASP:N	6:7:447:GLY:HA2	2.10	0.64
1:2:631:ILE:N	1:2:638:THR:O	2.25	0.64
5:6:355:ASP:CB	5:6:382:ARG:HA	2.27	0.64
6:7:249:SER:CA	6:7:507:ILE:HA	2.24	0.64
5:6:326:LYS:H	5:6:327:TYR:HA	1.62	0.64
5:6:765:LEU:CB	5:6:819:ILE:H	2.11	0.64
1:2:327:ARG:O	1:2:591:LEU:N	2.25	0.64
2:3:203:ALA:O	2:3:207:GLY:N	2.31	0.64
6:7:499:LYS:HA	6:7:506:MET:N	2.13	0.63
2:3:449:ASP:CA	2:3:455:ARG:HA	2.27	0.63
3:4:761:ILE:O	3:4:816:VAL:HA	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:257:THR:HA	2:3:275:ASP:HA	1.79	0.63
2:3:191:LEU:O	2:3:454:GLU:HA	1.98	0.63
4:5:175:ARG:O	4:5:251:ILE:N	2.32	0.63
4:5:53:ASN:O	4:5:58:ASN:N	2.22	0.63
6:7:78:VAL:N	6:7:201:PHE:O	2.30	0.63
6:7:411:TYR:O	6:7:415:ALA:HB2	1.98	0.63
2:3:113:GLY:O	2:3:117:GLU:N	2.26	0.63
7:C:18:ILE:N	7:C:44:LEU:O	2.31	0.63
3:4:206:ARG:O	3:4:211:GLU:N	2.30	0.63
2:3:389:VAL:O	2:3:401:GLY:HA3	1.99	0.63
4:5:169:THR:O	4:5:463:TYR:HA	1.98	0.63
2:3:422:VAL:O	2:3:426:ALA:HB2	1.99	0.62
5:6:189:VAL:O	5:6:193:ALA:N	2.31	0.62
5:6:301:ARG:N	5:6:355:ASP:O	2.32	0.62
1:2:337:VAL:O	1:2:351:PHE:N	2.25	0.62
3:4:855:SER:HA	3:4:856:VAL:C	2.19	0.62
5:6:304:LEU:O	5:6:306:LYS:N	2.30	0.62
3:4:679:GLY:HA3	3:4:681:ARG:O	1.99	0.62
7:C:372:VAL:N	7:C:384:ASN:O	2.29	0.62
1:2:631:ILE:O	1:2:637:VAL:HA	1.99	0.62
2:3:453:GLY:N	6:7:366:LEU:O	2.32	0.62
1:2:332:PRO:O	1:2:383:ARG:HA	1.98	0.62
3:4:626:GLY:N	3:4:668:ARG:O	2.22	0.62
5:6:631:ALA:O	5:6:634:GLY:N	2.33	0.62
7:C:33:VAL:O	7:C:37:LEU:CB	2.47	0.62
3:4:352:CYS:N	3:4:353:ASP:HA	2.15	0.62
5:6:307:ALA:O	5:6:319:ASP:HA	1.99	0.62
5:6:663:ILE:N	5:6:670:ALA:O	2.33	0.62
6:7:457:CYS:N	6:7:596:ILE:O	2.22	0.62
3:4:408:ASP:C	3:4:410:GLN:H	2.03	0.61
3:4:605:ILE:H	3:4:617:GLU:H	1.47	0.61
5:6:155:TYR:N	5:6:268:PHE:O	2.24	0.61
6:7:312:GLU:HA	6:7:503:THR:CB	2.30	0.61
6:7:310:PHE:HA	6:7:336:ASN:HA	1.81	0.61
6:7:335:VAL:H	6:7:503:THR:CB	2.13	0.61
3:4:341:ASP:H	3:4:392:ALA:N	1.98	0.61
6:7:260:TYR:HA	6:7:300:MET:HA	1.82	0.61
1:2:568:GLY:HA2	1:2:607:ASP:O	2.01	0.61
2:3:61:ASP:C	6:7:213:ARG:HA	2.20	0.61
6:7:334:HIS:O	6:7:378:ALA:N	2.30	0.61
3:4:761:ILE:N	3:4:815:ASN:O	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:358:LYS:HA	5:6:380:ILE:HA	1.82	0.61
5:6:607:GLY:HA2	5:6:627:ALA:H	1.66	0.61
1:2:427:THR:O	1:2:454:ASN:N	2.34	0.61
3:4:245:ALA:HB3	3:4:306:TYR:O	2.01	0.61
3:4:442:ILE:N	3:4:458:LYS:O	2.24	0.61
3:4:648:VAL:O	3:4:652:GLN:N	2.29	0.61
3:4:917:ILE:C	3:4:927:VAL:HA	2.21	0.61
2:3:404:ASN:O	2:3:544:ASP:N	2.33	0.61
5:6:632:ASP:HA	5:6:675:ARG:O	2.00	0.61
1:2:660:THR:O	1:2:850:LYS:HA	2.01	0.60
3:4:917:ILE:O	3:4:927:VAL:HA	2.01	0.60
1:2:223:GLY:H	7:C:86:ASP:CB	2.14	0.60
1:2:327:ARG:N	1:2:591:LEU:N	2.49	0.60
4:5:175:ARG:O	4:5:250:PHE:HA	2.00	0.60
1:2:244:VAL:O	1:2:298:SER:N	2.34	0.60
2:3:314:LEU:CB	4:5:459:THR:H	2.15	0.60
5:6:134:LYS:N	5:6:135:VAL:HA	2.15	0.60
5:6:704:PRO:O	5:6:707:SER:N	2.34	0.60
2:3:669:PRO:O	2:3:720:THR:HA	2.02	0.60
1:2:821:ALA:O	1:2:825:LEU:N	2.34	0.60
2:3:462:MET:O	2:3:466:ASP:N	2.34	0.60
7:C:155:TYR:H	7:C:256:ASN:HA	1.66	0.60
1:2:576:LEU:HA	1:2:595:ALA:H	1.66	0.60
5:6:344:TRP:CB	5:6:345:THR:HA	2.31	0.60
5:6:509:SER:O	5:6:511:ASP:N	2.35	0.60
7:C:93:ILE:HA	7:C:150:THR:O	2.02	0.60
3:4:919:LEU:O	3:4:923:VAL:O	2.20	0.60
5:6:512:GLU:O	5:6:514:ASN:N	2.35	0.60
7:C:572:HIS:O	7:C:579:LYS:N	2.30	0.60
3:4:394:LYS:CB	3:4:420:TYR:HA	2.31	0.59
3:4:913:GLU:C	3:4:915:LYS:H	2.06	0.59
6:7:486:LYS:N	6:7:487:GLY:HA3	2.17	0.59
5:6:153:ILE:O	5:6:268:PHE:N	2.34	0.59
5:6:578:SER:HA	5:6:581:LYS:CA	2.31	0.59
6:7:372:THR:C	6:7:374:THR:H	2.06	0.59
4:5:182:MET:HA	4:5:189:THR:HA	1.84	0.59
5:6:663:ILE:O	5:6:670:ALA:N	2.26	0.59
1:2:631:ILE:O	1:2:638:THR:N	2.29	0.59
5:6:309:PHE:N	5:6:317:ILE:HA	2.18	0.59
6:7:465:ALA:O	6:7:468:GLN:N	2.34	0.59
3:4:188:GLN:C	3:4:190:CYS:H	2.05	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:408:VAL:O	2:3:549:VAL:N	2.29	0.59
2:3:500:ALA:H	2:3:501:GLY:HA3	1.67	0.59
3:4:241:LEU:O	3:4:303:VAL:HA	2.02	0.59
5:6:360:ARG:HA	5:6:378:ASP:HA	1.85	0.59
1:2:356:ASN:N	1:2:434:TYR:O	2.36	0.58
1:2:328:THR:HA	1:2:589:TRP:O	2.03	0.58
6:7:258:ILE:N	6:7:271:GLN:O	2.34	0.58
1:2:333:GLN:HA	1:2:383:ARG:HA	1.85	0.58
6:7:311:GLN:HA	6:7:504:ASP:C	2.24	0.58
1:2:428:GLY:HA2	1:2:453:ALA:HA	1.84	0.58
3:4:656:ILE:N	3:4:663:THR:O	2.37	0.58
1:2:547:THR:C	1:2:549:LYS:N	2.56	0.58
2:3:686:LEU:O	2:3:690:ASP:CB	2.52	0.58
5:6:598:THR:O	5:6:639:ASP:N	2.21	0.58
3:4:546:GLY:HA2	3:4:807:ALA:HB2	1.86	0.58
7:C:155:TYR:N	7:C:256:ASN:HA	2.18	0.58
4:5:398:LYS:O	4:5:405:ARG:HA	2.03	0.58
3:4:534:GLU:O	3:4:537:LYS:N	2.37	0.58
5:6:557:LYS:HA	5:6:564:LYS:HA	1.85	0.58
2:3:237:GLU:O	2:3:239:ASN:N	2.37	0.57
3:4:233:MET:O	3:4:237:GLY:N	2.32	0.57
3:4:891:ASN:O	3:4:894:SER:HA	2.03	0.57
3:4:911:GLN:HA	3:4:916:VAL:O	2.04	0.57
6:7:608:ASP:O	6:7:611:LYS:N	2.37	0.57
2:3:432:THR:O	2:3:473:ASP:N	2.33	0.57
5:6:549:LEU:O	5:6:552:LEU:N	2.37	0.57
5:6:659:GLN:O	5:6:674:ALA:N	2.36	0.57
5:6:780:LEU:O	5:6:784:ASP:N	2.28	0.57
6:7:257:VAL:HA	6:7:272:GLU:HA	1.86	0.57
7:C:39:GLN:O	7:C:213:ALA:HB1	2.04	0.57
1:2:575:GLY:C	1:2:577:THR:H	2.07	0.57
1:2:575:GLY:O	1:2:577:THR:N	2.37	0.57
3:4:609:VAL:HA	3:4:612:LYS:HA	1.86	0.57
4:5:181:ILE:N	4:5:190:THR:O	2.28	0.57
6:7:685:THR:O	6:7:688:THR:N	2.37	0.57
5:6:501:GLN:O	5:6:504:PHE:N	2.36	0.57
3:4:917:ILE:H	3:4:927:VAL:CA	2.18	0.57
4:5:175:ARG:N	4:5:251:ILE:O	2.37	0.57
2:3:675:ALA:O	2:3:678:VAL:N	2.38	0.57
3:4:629:CYS:N	3:4:670:SER:O	2.36	0.57
6:7:395:SER:C	6:7:397:VAL:H	2.08	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:344:VAL:HA	3:4:359:GLU:HA	1.86	0.56
6:7:335:VAL:N	6:7:503:THR:CB	2.68	0.56
1:2:477:THR:O	1:2:481:GLU:N	2.28	0.56
5:6:543:VAL:O	5:6:546:GLY:N	2.38	0.56
6:7:521:CYS:N	6:7:562:SER:O	2.37	0.56
1:2:632:SER:HA	1:2:637:VAL:HA	1.87	0.56
4:5:475:GLY:O	4:5:517:THR:HA	2.06	0.56
5:6:291:SER:HA	5:6:396:LYS:HA	1.87	0.56
5:6:554:GLY:O	5:6:567:GLY:HA2	2.05	0.56
6:7:310:PHE:O	6:7:504:ASP:O	2.23	0.56
6:7:498:MET:C	6:7:507:ILE:H	2.09	0.56
7:C:349:SER:O	7:C:352:LYS:N	2.39	0.56
3:4:567:CYS:O	3:4:708:VAL:N	2.37	0.56
5:6:607:GLY:CA	5:6:627:ALA:N	2.69	0.56
5:6:811:ALA:O	5:6:815:CYS:N	2.38	0.56
6:7:247:ARG:O	6:7:508:LEU:N	2.38	0.56
1:2:290:HIS:O	1:2:292:GLU:N	2.39	0.56
3:4:440:ARG:O	3:4:460:TYR:N	2.39	0.56
4:5:500:GLN:O	4:5:515:SER:N	2.33	0.56
1:2:332:PRO:C	1:2:383:ARG:HA	2.27	0.55
1:2:395:GLY:HA2	1:2:561:HIS:O	2.06	0.55
3:4:855:SER:HA	3:4:857:ILE:N	2.21	0.55
7:C:137:ALA:O	7:C:140:GLN:N	2.39	0.55
3:4:602:THR:N	3:4:619:GLY:HA3	2.22	0.55
5:6:135:VAL:O	5:6:138:ALA:N	2.39	0.55
5:6:754:TYR:O	5:6:757:TYR:N	2.40	0.55
7:C:522:SER:HA	7:C:525:ARG:CB	2.37	0.55
4:5:455:ARG:HA	4:5:462:PHE:HA	1.88	0.55
3:4:601:LEU:O	3:4:621:LEU:N	2.33	0.55
4:5:613:ARG:N	4:5:670:PRO:O	2.39	0.55
7:C:351:MET:C	7:C:353:ARG:N	2.59	0.55
2:3:202:TYR:N	2:3:242:THR:O	2.26	0.55
6:7:467:SER:O	6:7:470:LEU:N	2.39	0.55
5:6:763:PRO:HA	5:6:817:ASP:C	2.27	0.55
6:7:247:ARG:N	6:7:509:GLU:HA	2.18	0.55
1:2:702:SER:O	1:2:705:ARG:N	2.39	0.55
5:6:310:THR:C	5:6:345:THR:H	2.09	0.55
6:7:209:GLN:H	6:7:212:ALA:CB	2.20	0.55
6:7:262:CYS:C	6:7:264:GLN:H	2.11	0.55
7:C:205:ILE:CA	7:C:251:ILE:HA	2.36	0.55
5:6:126:SER:O	5:6:132:VAL:HA	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:525:ILE:HA	5:6:528:LYS:H	1.71	0.55
1:2:566:ALA:N	1:2:605:LEU:O	2.26	0.54
5:6:580:SER:O	5:6:581:LYS:C	2.45	0.54
3:4:540:ILE:O	3:4:543:GLN:N	2.40	0.54
4:5:266:PRO:C	4:5:268:GLY:H	2.10	0.54
5:6:404:VAL:N	5:6:451:LYS:O	2.37	0.54
6:7:686:PRO:O	6:7:689:LEU:N	2.41	0.54
2:3:441:GLY:HA2	2:3:461:ALA:N	2.22	0.54
3:4:677:PRO:O	3:4:680:SER:HA	2.07	0.54
5:6:303:GLU:H	5:6:354:LEU:N	2.03	0.54
3:4:594:LYS:C	3:4:596:SER:H	2.09	0.54
5:6:695:LEU:O	5:6:699:LEU:N	2.34	0.54
2:3:297:VAL:O	2:3:321:ILE:HA	2.06	0.54
3:4:334:ARG:O	3:4:398:LYS:N	2.38	0.54
5:6:794:ARG:N	5:6:795:ILE:HA	2.14	0.54
1:2:279:THR:O	1:2:283:TYR:N	2.29	0.54
3:4:832:ALA:O	3:4:836:TYR:N	2.41	0.54
6:7:460:GLY:HA3	6:7:600:MET:O	2.07	0.54
1:2:556:VAL:O	1:2:559:THR:N	2.41	0.54
3:4:517:ASP:O	3:4:520:SER:N	2.41	0.54
4:5:52:ASN:O	4:5:56:VAL:N	2.30	0.54
5:6:164:GLY:O	5:6:168:MET:N	2.30	0.54
7:C:204:ALA:HB1	7:C:252:ASP:C	2.27	0.54
3:4:341:ASP:H	3:4:392:ALA:H	1.55	0.54
5:6:661:ILE:O	5:6:672:LEU:N	2.38	0.54
7:C:78:THR:O	7:C:92:TYR:HA	2.07	0.54
2:3:432:THR:N	2:3:471:CYS:O	2.32	0.54
3:4:688:VAL:O	3:4:691:ASN:N	2.40	0.54
3:4:795:THR:O	3:4:798:LEU:N	2.41	0.54
4:5:544:THR:O	4:5:547:LEU:N	2.41	0.54
6:7:25:LEU:C	6:7:27:THR:N	2.61	0.54
6:7:619:VAL:HA	6:7:622:HIS:O	2.08	0.54
2:3:95:ARG:HA	2:3:154:LYS:O	2.08	0.54
5:6:308:SER:HA	5:6:318:VAL:O	2.08	0.54
2:3:437:SER:CB	2:3:438:SER:HA	2.38	0.53
4:5:441:GLY:HA3	4:5:443:GLY:N	2.23	0.53
5:6:607:GLY:HA2	5:6:627:ALA:N	2.23	0.53
1:2:386:GLN:O	1:2:409:ILE:CA	2.55	0.53
2:3:188:LYS:CA	2:3:458:GLU:HA	2.34	0.53
4:5:729:SER:O	4:5:731:GLN:N	2.40	0.53
5:6:586:LYS:O	5:6:589:VAL:N	2.40	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:68:GLN:HA	6:7:71:ALA:HB3	1.89	0.53
7:C:34:ARG:O	7:C:38:LEU:N	2.39	0.53
1:2:258:LEU:O	1:2:261:ALA:N	2.41	0.53
3:4:434:GLU:N	3:4:467:LYS:O	2.30	0.53
4:5:60:SER:HA	4:5:136:GLN:O	2.08	0.53
6:7:444:VAL:N	6:7:448:MET:O	2.42	0.53
1:2:777:LYS:O	1:2:828:PHE:HA	2.08	0.53
1:2:860:SER:O	1:2:864:TYR:N	2.42	0.53
5:6:559:THR:N	5:6:565:LEU:H	2.07	0.53
5:6:791:SER:HA	5:6:839:ASP:HA	1.88	0.53
1:2:333:GLN:HA	1:2:383:ARG:CB	2.38	0.53
2:3:377:ILE:O	2:3:380:ALA:HB3	2.08	0.53
3:4:833:ILE:C	3:4:836:TYR:H	2.12	0.53
4:5:33:ASN:O	4:5:37:GLU:N	2.40	0.53
4:5:170:SER:H	4:5:256:LEU:HA	1.73	0.53
5:6:777:TYR:O	5:6:780:LEU:N	2.36	0.53
3:4:915:LYS:HA	3:4:931:ASN:O	2.08	0.53
5:6:291:SER:HA	5:6:395:CYS:O	2.09	0.53
5:6:518:GLU:O	5:6:522:ASP:N	2.38	0.53
5:6:725:THR:O	5:6:728:ALA:HB3	2.08	0.53
2:3:452:THR:CA	6:7:368:ALA:H	2.18	0.53
2:3:183:GLU:HA	2:3:293:ASN:HA	1.90	0.53
4:5:627:VAL:O	4:5:631:LYS:CB	2.56	0.53
5:6:334:PRO:O	5:6:339:GLU:HA	2.08	0.53
1:2:699:VAL:O	1:2:702:SER:N	2.42	0.53
7:C:373:VAL:HA	7:C:383:MET:HA	1.91	0.53
3:4:397:ILE:O	3:4:416:SER:HA	2.09	0.53
1:2:244:VAL:H	1:2:297:ILE:C	2.12	0.52
2:3:270:LEU:HA	4:5:510:THR:H	1.75	0.52
5:6:151:ILE:O	5:6:266:SER:N	2.42	0.52
7:C:103:ASP:O	7:C:105:LYS:N	2.42	0.52
3:4:854:LYS:N	3:4:857:ILE:CB	2.72	0.52
3:4:917:ILE:H	3:4:927:VAL:HA	1.72	0.52
2:3:245:TYR:C	2:3:247:TYR:H	2.13	0.52
6:7:208:SER:O	6:7:212:ALA:HB2	2.10	0.52
3:4:608:ASP:C	3:4:610:ASP:H	2.12	0.52
6:7:457:CYS:O	6:7:598:PHE:N	2.36	0.52
7:C:206:ARG:CB	7:C:221:SER:H	2.23	0.52
7:C:344:LEU:O	7:C:348:SER:CB	2.57	0.52
4:5:598:LYS:O	4:5:601:ARG:N	2.43	0.52
6:7:353:GLY:HA3	6:7:377:GLU:O	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:751:LEU:O	5:6:754:TYR:N	2.43	0.52
5:6:764:ILE:CB	5:6:765:LEU:HA	2.40	0.52
6:7:245:ILE:O	6:7:346:GLY:N	2.42	0.52
1:2:600:ASP:C	1:2:602:GLY:H	2.13	0.52
2:3:392:ASN:HA	2:3:398:HIS:HA	1.91	0.52
3:4:563:ASN:O	3:4:703:ASP:N	2.43	0.52
6:7:700:ALA:HB1	6:7:705:ALA:CB	2.40	0.52
3:4:721:ALA:O	3:4:725:THR:CB	2.58	0.52
5:6:525:ILE:O	5:6:528:LYS:N	2.43	0.52
5:6:773:LEU:O	5:6:776:LYS:N	2.42	0.52
5:6:816:VAL:N	5:6:817:ASP:HA	2.24	0.52
1:2:347:ILE:C	1:2:349:GLY:H	2.12	0.52
1:2:663:LEU:O	1:2:667:VAL:N	2.42	0.52
2:3:197:ILE:N	2:3:249:THR:O	2.42	0.52
3:4:588:GLY:HA2	3:4:628:VAL:O	2.10	0.52
3:4:917:ILE:H	3:4:927:VAL:CB	2.23	0.52
4:5:458:MET:C	4:5:460:ARG:H	2.14	0.52
4:5:717:GLU:O	4:5:721:ARG:CB	2.58	0.52
4:5:753:TYR:O	4:5:757:LYS:CB	2.58	0.52
5:6:661:ILE:H	5:6:672:LEU:C	2.13	0.52
6:7:628:LEU:N	6:7:629:ASP:HA	2.24	0.52
1:2:327:ARG:HA	1:2:388:VAL:HA	1.92	0.51
2:3:723:LYS:O	2:3:726:ALA:HB3	2.10	0.51
4:5:596:ILE:HA	4:5:599:MET:CB	2.41	0.51
1:2:674:LEU:O	1:2:677:PHE:N	2.43	0.51
1:2:321:THR:HA	1:2:425:GLU:HA	1.91	0.51
6:7:512:ALA:O	6:7:516:ALA:N	2.33	0.51
7:C:327:LEU:O	7:C:331:SER:CB	2.58	0.51
2:3:197:ILE:O	2:3:249:THR:O	2.29	0.51
2:3:411:PRO:C	2:3:413:THR:H	2.14	0.51
6:7:713:VAL:O	6:7:716:ALA:N	2.43	0.51
1:2:433:ASN:HA	1:2:434:TYR:CB	2.40	0.51
5:6:361:ILE:N	5:6:377:LEU:O	2.42	0.51
3:4:657:ALA:HA	3:4:662:ILE:HA	1.92	0.51
1:2:327:ARG:O	1:2:590:THR:HA	2.10	0.51
1:2:599:ALA:O	1:2:602:GLY:N	2.44	0.51
3:4:188:GLN:C	3:4:190:CYS:N	2.64	0.51
5:6:523:GLU:O	5:6:525:ILE:N	2.37	0.51
5:6:608:LEU:N	5:6:625:ALA:HA	2.25	0.51
6:7:314:LYS:HA	6:7:331:LEU:O	2.11	0.51
2:3:195:LYS:HA	6:7:371:LEU:C	2.31	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:197:ILE:CA	2:3:249:THR:O	2.59	0.51
3:4:608:ASP:O	3:4:610:ASP:N	2.43	0.51
6:7:214:ARG:N	6:7:215:TYR:HA	2.25	0.51
7:C:198:ILE:HA	7:C:229:LEU:O	2.11	0.51
7:C:519:ILE:O	7:C:523:LEU:CB	2.58	0.51
3:4:566:LEU:HA	3:4:706:TYR:O	2.10	0.51
4:5:757:LYS:C	4:5:759:GLU:H	2.14	0.51
5:6:721:GLU:O	5:6:725:THR:CB	2.59	0.51
1:2:629:ILE:O	1:2:639:THR:HA	2.10	0.51
3:4:393:ASP:O	3:4:394:LYS:C	2.50	0.51
2:3:270:LEU:CB	4:5:509:ILE:HA	2.41	0.51
6:7:357:PRO:HA	6:7:374:THR:CA	2.40	0.51
6:7:417:SER:CB	6:7:633:VAL:H	2.24	0.51
7:C:103:ASP:C	7:C:105:LYS:H	2.14	0.51
1:2:223:GLY:HA2	7:C:86:ASP:N	2.26	0.51
3:4:378:GLU:C	3:4:380:ASN:N	2.64	0.50
7:C:37:LEU:HA	7:C:41:ASP:HA	1.92	0.50
5:6:541:GLU:O	5:6:544:LYS:N	2.44	0.50
6:7:483:THR:N	6:7:522:CYS:O	2.41	0.50
2:3:346:ASP:O	2:3:349:ASN:N	2.44	0.50
5:6:641:PHE:O	5:6:644:MET:CB	2.59	0.50
3:4:888:LYS:O	3:4:892:GLU:CB	2.59	0.50
3:4:592:SER:HA	3:4:632:ASP:CB	2.41	0.50
4:5:54:ILE:O	4:5:57:LYS:N	2.39	0.50
4:5:664:ALA:O	4:5:668:LEU:N	2.45	0.50
5:6:661:ILE:O	5:6:671:THR:HA	2.12	0.50
5:6:600:GLY:H	5:6:639:ASP:CB	2.24	0.50
1:2:663:LEU:O	1:2:666:ASN:N	2.44	0.50
5:6:141:GLU:O	5:6:144:LYS:N	2.45	0.50
4:5:180:SER:HA	4:5:191:SER:HA	1.92	0.50
5:6:334:PRO:C	5:6:339:GLU:HA	2.32	0.49
5:6:397:PHE:HA	5:6:458:HIS:O	2.12	0.49
5:6:835:ILE:O	5:6:838:VAL:N	2.45	0.49
7:C:204:ALA:HB1	7:C:252:ASP:O	2.12	0.49
7:C:92:TYR:O	7:C:151:LYS:HA	2.12	0.49
3:4:331:LEU:HA	3:4:431:ASP:O	2.12	0.49
6:7:256:GLU:N	6:7:306:LYS:O	2.31	0.49
6:7:446:ASP:N	6:7:447:GLY:CA	2.75	0.49
1:2:388:VAL:N	1:2:408:VAL:O	2.39	0.49
6:7:590:LEU:O	6:7:593:ARG:N	2.45	0.49
3:4:727:LEU:HA	3:4:728:TYR:C	2.32	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:289:ILE:C	1:2:291:SER:H	2.16	0.49
3:4:571:SER:C	3:4:573:SER:H	2.16	0.49
2:3:173:ALA:HB1	4:5:250:PHE:O	2.12	0.49
5:6:523:GLU:C	5:6:525:ILE:H	2.15	0.49
5:6:401:GLU:O	5:6:454:PHE:HA	2.13	0.49
6:7:253:PRO:HA	6:7:308:SER:O	2.13	0.49
4:5:612:PRO:HA	4:5:670:PRO:HA	1.94	0.49
5:6:309:PHE:HA	5:6:345:THR:O	2.13	0.49
5:6:793:TYR:HA	5:6:794:ARG:HA	1.60	0.49
2:3:406:LEU:O	2:3:547:PHE:N	2.44	0.49
2:3:414:ALA:O	2:3:417:GLN:N	2.46	0.48
1:2:481:GLU:O	1:2:484:PHE:N	2.45	0.48
2:3:190:SER:N	2:3:456:ARG:HA	2.28	0.48
6:7:480:GLY:HA2	6:7:520:ILE:O	2.13	0.48
1:2:357:GLU:N	1:2:435:ASP:CB	2.77	0.48
4:5:186:CYS:C	4:5:188:HIS:H	2.16	0.48
4:5:169:THR:O	4:5:462:PHE:O	2.31	0.48
5:6:529:LEU:O	5:6:532:SER:N	2.45	0.48
1:2:510:ASP:O	1:2:513:THR:N	2.46	0.48
3:4:202:LYS:CA	3:4:224:LEU:HA	2.40	0.48
4:5:107:ALA:O	4:5:109:SER:HA	2.13	0.48
6:7:546:ILE:O	6:7:557:LEU:N	2.47	0.48
7:C:324:VAL:O	7:C:327:LEU:N	2.47	0.48
1:2:222:THR:HA	7:C:87:VAL:N	2.29	0.48
1:2:242:LEU:O	1:2:295:VAL:HA	2.13	0.48
2:3:191:LEU:H	2:3:455:ARG:C	2.17	0.48
2:3:193:ARG:O	2:3:253:HIS:N	2.45	0.48
2:3:449:ASP:HA	2:3:455:ARG:CA	2.41	0.48
3:4:249:LEU:HA	3:4:250:ALA:HA	1.50	0.48
3:4:341:ASP:N	3:4:392:ALA:O	2.46	0.48
3:4:850:VAL:O	3:4:853:GLY:N	2.47	0.48
4:5:177:THR:O	4:5:193:THR:HA	2.14	0.48
5:6:574:VAL:O	5:6:715:ILE:N	2.46	0.48
1:2:547:THR:O	1:2:549:LYS:N	2.47	0.48
1:2:630:SER:HA	1:2:639:THR:CA	2.35	0.48
1:2:826:SER:C	1:2:828:PHE:H	2.17	0.48
3:4:645:LEU:O	3:4:648:VAL:N	2.47	0.48
4:5:450:THR:C	4:5:467:GLY:HA3	2.34	0.48
4:5:736:GLU:O	4:5:740:THR:N	2.44	0.48
5:6:288:LEU:N	5:6:399:GLY:HA3	2.29	0.48
4:5:729:SER:H	4:5:775:VAL:C	2.17	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:721:GLU:HA	5:6:724:ASP:CB	2.43	0.48
6:7:650:PRO:CA	6:7:706:ASP:HA	2.43	0.48
7:C:376:ASN:N	7:C:380:GLU:O	2.31	0.48
5:6:554:GLY:HA2	5:6:808:GLU:CB	2.43	0.47
1:2:333:GLN:HA	1:2:383:ARG:CA	2.44	0.47
4:5:297:ILE:N	4:5:329:LYS:O	2.33	0.47
7:C:328:ASN:HA	7:C:332:ARG:CB	2.44	0.47
4:5:441:GLY:HA3	4:5:443:GLY:H	1.78	0.47
5:6:802:SER:O	5:6:805:ARG:N	2.47	0.47
6:7:17:LEU:O	6:7:20:GLU:N	2.47	0.47
6:7:290:SER:C	6:7:292:ASN:H	2.18	0.47
5:6:661:ILE:C	5:6:672:LEU:H	2.17	0.47
6:7:580:PRO:C	6:7:582:ASP:H	2.18	0.47
2:3:294:VAL:HA	2:3:326:VAL:HA	1.96	0.47
3:4:651:GLN:C	3:4:653:THR:H	2.18	0.47
3:4:719:GLU:O	3:4:722:LYS:N	2.45	0.47
5:6:357:GLN:O	5:6:381:LEU:N	2.42	0.47
5:6:768:GLU:HA	5:6:769:ALA:HA	1.49	0.47
1:2:540:LEU:O	1:2:681:CYS:N	2.36	0.47
2:3:447:THR:HA	2:3:448:THR:HA	1.45	0.47
5:6:799:GLN:O	5:6:802:SER:N	2.47	0.47
6:7:249:SER:CB	6:7:505:GLU:C	2.83	0.47
6:7:493:LEU:HA	6:7:512:ALA:HB3	1.96	0.47
7:C:533:TYR:O	7:C:536:SER:N	2.48	0.47
5:6:601:LYS:CB	5:6:640:GLU:O	2.63	0.47
5:6:661:ILE:H	5:6:672:LEU:N	2.12	0.47
1:2:219:THR:CB	1:2:225:SER:HA	2.44	0.47
3:4:705:VAL:O	3:4:832:ALA:HB2	2.15	0.47
5:6:606:ALA:O	5:6:609:THR:N	2.47	0.47
6:7:250:ASP:CA	6:7:505:GLU:O	2.61	0.47
1:2:343:LYS:CB	1:2:371:GLY:HA3	2.45	0.47
1:2:528:ASN:HA	1:2:529:GLY:HA2	1.50	0.47
2:3:201:HIS:O	2:3:209:PHE:HA	2.15	0.47
3:4:913:GLU:C	3:4:915:LYS:N	2.65	0.47
4:5:540:ILE:O	4:5:543:GLN:N	2.47	0.47
6:7:102:LEU:O	6:7:106:ILE:N	2.37	0.47
6:7:680:SER:CB	6:7:681:PHE:HA	2.45	0.47
2:3:435:ARG:HA	2:3:436:GLY:HA3	1.62	0.47
5:6:399:GLY:O	5:6:400:VAL:C	2.53	0.47
5:6:913:MET:O	5:6:916:MET:N	2.48	0.47
6:7:334:HIS:HA	6:7:503:THR:CA	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:446:ASP:H	6:7:447:GLY:HA2	1.78	0.47
7:C:61:LEU:O	7:C:64:LYS:N	2.46	0.47
2:3:443:THR:C	2:3:445:ALA:H	2.18	0.47
2:3:462:MET:HA	2:3:465:ALA:HB3	1.97	0.47
1:2:386:GLN:CB	1:2:410:LEU:O	2.56	0.46
2:3:270:LEU:CB	4:5:510:THR:H	2.27	0.46
4:5:459:THR:C	4:5:460:ARG:O	2.54	0.46
7:C:407:ALA:O	7:C:410:TRP:N	2.47	0.46
2:3:500:ALA:N	2:3:501:GLY:HA3	2.29	0.46
3:4:603:ALA:H	3:4:619:GLY:H	1.63	0.46
4:5:408:GLY:HA2	4:5:409:ASP:HA	1.59	0.46
5:6:652:ILE:O	5:6:656:MET:N	2.31	0.46
2:3:188:LYS:O	2:3:457:LEU:C	2.54	0.46
2:3:187:THR:CB	2:3:459:ALA:H	2.29	0.46
4:5:448:GLY:O	4:5:467:GLY:HA2	2.15	0.46
6:7:717:LEU:O	6:7:720:VAL:N	2.49	0.46
6:7:78:VAL:O	6:7:203:TYR:N	2.32	0.46
1:2:219:THR:N	7:C:85:ASP:H	2.13	0.46
1:2:600:ASP:CB	1:2:642:ALA:HA	2.46	0.46
1:2:630:SER:HA	1:2:638:THR:O	2.15	0.46
2:3:18:ASP:O	2:3:21:PHE:N	2.49	0.46
7:C:307:LEU:CB	7:C:312:LYS:H	2.28	0.46
7:C:375:LEU:HA	7:C:381:LEU:HA	1.97	0.46
1:2:245:ASN:HA	1:2:298:SER:CB	2.46	0.46
1:2:385:TYR:CB	1:2:410:LEU:O	2.63	0.46
2:3:195:LYS:O	2:3:251:ILE:O	2.33	0.46
5:6:370:THR:HA	5:6:371:GLY:HA2	1.63	0.46
3:4:485:LEU:HA	7:C:575:ASP:CB	2.46	0.46
3:4:342:MET:HA	3:4:390:SER:O	2.16	0.46
4:5:54:ILE:C	4:5:57:LYS:H	2.17	0.46
1:2:333:GLN:O	1:2:334:LEU:CB	2.63	0.46
4:5:264:LEU:HA	4:5:265:VAL:HA	1.56	0.46
6:7:501:PRO:O	6:7:503:THR:N	2.49	0.46
6:7:547:SER:HA	6:7:556:THR:HA	1.96	0.46
1:2:652:PRO:O	1:2:653:ASN:C	2.54	0.46
4:5:502:ILE:N	4:5:513:LEU:O	2.41	0.46
5:6:326:LYS:N	5:6:327:TYR:HA	2.30	0.46
6:7:312:GLU:CB	6:7:504:ASP:HA	2.45	0.46
1:2:242:LEU:N	1:2:294:HIS:O	2.42	0.46
2:3:449:ASP:HA	2:3:454:GLU:C	2.36	0.46
5:6:310:THR:N	5:6:317:ILE:H	2.12	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:349:VAL:HA	6:7:383:GLN:HA	1.97	0.46
1:2:322:GLY:O	1:2:423:GLU:HA	2.15	0.45
2:3:562:SER:CB	4:5:623:SER:HA	2.45	0.45
3:4:242:ASN:O	3:4:305:PRO:HA	2.16	0.45
3:4:577:ILE:O	3:4:580:TYR:N	2.49	0.45
6:7:247:ARG:H	6:7:509:GLU:CA	2.23	0.45
6:7:251:VAL:HA	6:7:310:PHE:O	2.16	0.45
7:C:208:LYS:HA	7:C:219:TRP:HA	1.98	0.45
1:2:224:ARG:O	1:2:226:VAL:N	2.50	0.45
4:5:209:ARG:HA	4:5:239:ASP:CB	2.45	0.45
5:6:608:LEU:H	5:6:625:ALA:HA	1.81	0.45
1:2:327:ARG:H	1:2:591:LEU:H	1.64	0.45
2:3:666:ARG:HA	2:3:667:VAL:HA	1.72	0.45
6:7:106:ILE:O	6:7:110:ALA:HB2	2.17	0.45
1:2:327:ARG:C	1:2:591:LEU:H	2.16	0.45
1:2:776:PRO:HA	1:2:827:GLU:CA	2.46	0.45
2:3:418:LEU:O	2:3:421:PHE:N	2.49	0.45
3:4:854:LYS:H	3:4:857:ILE:CB	2.30	0.45
4:5:108:GLN:HA	4:5:109:SER:HA	1.69	0.45
7:C:211:THR:H	7:C:247:SER:HA	1.82	0.45
3:4:245:ALA:HA	3:4:246:ARG:HA	1.52	0.45
4:5:616:PRO:O	4:5:619:ALA:HB3	2.16	0.45
5:6:601:LYS:CB	5:6:644:MET:N	2.79	0.45
1:2:268:LEU:O	1:2:271:PHE:N	2.50	0.45
1:2:359:ILE:HA	1:2:360:ARG:HA	1.60	0.45
1:2:329:GLY:N	1:2:589:TRP:O	2.50	0.45
3:4:339:ILE:O	3:4:392:ALA:O	2.35	0.45
3:4:854:LYS:C	3:4:857:ILE:H	2.08	0.45
4:5:53:ASN:O	4:5:57:LYS:N	2.49	0.45
5:6:308:SER:C	5:6:317:ILE:HA	2.37	0.45
5:6:654:GLU:O	5:6:657:GLU:N	2.45	0.45
5:6:659:GLN:CB	5:6:674:ALA:HB3	2.46	0.45
6:7:224:PRO:HA	6:7:241:VAL:HA	1.98	0.45
4:5:439:THR:O	4:5:479:ILE:HA	2.17	0.45
5:6:356:TRP:HA	5:6:381:LEU:O	2.16	0.45
5:6:559:THR:N	5:6:563:ILE:O	2.50	0.45
2:3:429:ALA:HB3	2:3:469:VAL:O	2.17	0.45
4:5:258:LEU:N	4:5:274:LEU:O	2.49	0.45
1:2:280:GLU:HA	1:2:283:TYR:O	2.17	0.45
3:4:502:THR:O	3:4:505:ASP:N	2.50	0.45
4:5:266:PRO:O	4:5:268:GLY:N	2.39	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:405:PRO:CA	5:6:450:TYR:HA	2.36	0.45
2:3:449:ASP:HA	2:3:454:GLU:O	2.17	0.44
4:5:413:LEU:HA	4:5:521:ALA:O	2.17	0.44
5:6:723:ILE:O	5:6:726:GLU:N	2.50	0.44
6:7:315:ILE:O	6:7:331:LEU:N	2.49	0.44
6:7:517:ASP:C	6:7:519:GLY:H	2.20	0.44
1:2:224:ARG:O	1:2:225:SER:C	2.54	0.44
1:2:318:VAL:N	1:2:428:GLY:O	2.26	0.44
2:3:301:LEU:O	2:3:318:LYS:O	2.35	0.44
5:6:545:LYS:O	5:6:548:LEU:N	2.51	0.44
5:6:605:ALA:C	5:6:607:GLY:N	2.70	0.44
6:7:311:GLN:O	6:7:503:THR:CB	2.65	0.44
2:3:406:LEU:N	2:3:545:LEU:O	2.50	0.44
2:3:690:ASP:O	2:3:693:LYS:N	2.51	0.44
3:4:822:VAL:O	3:4:825:ALA:HB3	2.18	0.44
6:7:310:PHE:C	6:7:504:ASP:O	2.55	0.44
6:7:369:GLY:HA2	6:7:370:LEU:HA	1.56	0.44
6:7:428:VAL:O	6:7:431:ALA:HB3	2.17	0.44
5:6:310:THR:O	5:6:345:THR:N	2.46	0.44
6:7:655:ALA:O	6:7:658:ASP:N	2.50	0.44
2:3:684:THR:O	2:3:688:ASN:CB	2.66	0.44
3:4:800:SER:O	3:4:801:MET:C	2.55	0.44
4:5:95:THR:HA	4:5:98:ALA:HB3	2.00	0.44
6:7:334:HIS:HA	6:7:503:THR:CB	2.48	0.44
7:C:373:VAL:HA	7:C:382:THR:O	2.18	0.44
5:6:305:TYR:CB	5:6:352:ARG:CB	2.96	0.44
5:6:313:MET:HA	5:6:314:CYS:HA	1.49	0.44
3:4:733:PRO:CB	6:7:445:GLY:N	2.71	0.44
6:7:209:GLN:H	6:7:212:ALA:H	1.65	0.44
5:6:624:GLU:O	5:6:626:GLY:N	2.51	0.44
6:7:251:VAL:HA	6:7:504:ASP:O	2.18	0.44
2:3:530:HIS:C	2:3:532:ASN:H	2.20	0.44
7:C:574:VAL:N	7:C:577:GLY:O	2.25	0.44
3:4:760:PRO:HA	3:4:815:ASN:HA	2.00	0.43
6:7:109:ASN:C	6:7:111:ASN:H	2.21	0.43
6:7:250:ASP:N	6:7:506:MET:O	2.51	0.43
1:2:629:ILE:N	1:2:640:LEU:O	2.39	0.43
3:4:910:LEU:O	3:4:915:LYS:N	2.51	0.43
5:6:304:LEU:C	5:6:306:LYS:N	2.72	0.43
5:6:287:LEU:HA	5:6:400:VAL:H	1.83	0.43
6:7:531:GLU:O	6:7:534:ARG:N	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:685:ASN:C	3:4:686:LEU:O	2.52	0.43
5:6:133:GLU:CB	5:6:134:LYS:HA	2.47	0.43
5:6:641:PHE:N	5:6:681:ALA:O	2.45	0.43
7:C:377:SER:C	7:C:379:GLY:H	2.21	0.43
2:3:412:SER:C	2:3:414:ALA:H	2.22	0.43
3:4:804:LEU:O	3:4:807:ALA:N	2.51	0.43
1:2:331:PHE:O	1:2:384:ASN:CA	2.59	0.43
2:3:29:GLN:N	2:3:31:PHE:O	2.52	0.43
2:3:404:ASN:HA	2:3:512:VAL:O	2.19	0.43
3:4:336:THR:N	3:4:396:VAL:O	2.46	0.43
5:6:505:LEU:O	5:6:509:SER:N	2.33	0.43
5:6:524:HIS:O	5:6:526:TYR:N	2.52	0.43
1:2:524:PRO:CB	1:2:525:LYS:HA	2.48	0.43
1:2:600:ASP:HA	1:2:643:ARG:H	1.83	0.43
3:4:501:ILE:O	3:4:502:THR:C	2.54	0.43
4:5:331:LEU:HA	4:5:332:GLY:HA2	1.63	0.43
5:6:802:SER:O	5:6:803:MET:C	2.56	0.43
2:3:223:THR:H	4:5:246:GLU:HA	1.82	0.43
5:6:123:SER:CB	5:6:135:VAL:H	2.32	0.43
6:7:724:LYS:C	6:7:726:SER:H	2.22	0.43
7:C:237:ALA:O	7:C:241:GLN:N	2.52	0.43
7:C:206:ARG:N	7:C:251:ILE:HA	2.33	0.43
2:3:236:THR:HA	2:3:237:GLU:C	2.39	0.43
2:3:711:ALA:O	2:3:714:LYS:N	2.52	0.43
3:4:593:GLY:C	3:4:595:GLY:H	2.22	0.43
3:4:833:ILE:O	3:4:836:TYR:N	2.49	0.43
5:6:764:ILE:C	5:6:818:GLU:HA	2.39	0.43
6:7:2:SER:C	6:7:4:ALA:H	2.22	0.43
3:4:408:ASP:C	3:4:410:GLN:N	2.68	0.43
3:4:738:GLN:HA	3:4:739:ASP:HA	1.70	0.43
4:5:235:ASN:HA	4:5:236:CYS:HA	1.87	0.43
4:5:499:GLN:C	4:5:501:THR:H	2.22	0.43
5:6:653:HIS:O	5:6:657:GLU:N	2.51	0.43
6:7:395:SER:O	6:7:397:VAL:N	2.50	0.43
6:7:616:VAL:O	6:7:619:VAL:O	2.37	0.43
5:6:309:PHE:CA	5:6:317:ILE:HA	2.48	0.43
6:7:262:CYS:O	6:7:264:GLN:N	2.50	0.43
6:7:672:LYS:O	6:7:675:MET:N	2.48	0.43
6:7:701:LYS:C	6:7:704:LEU:H	2.22	0.43
7:C:386:PRO:O	7:C:388:ARG:N	2.51	0.43
1:2:244:VAL:H	1:2:297:ILE:CA	2.32	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:826:SER:O	1:2:828:PHE:N	2.51	0.42
2:3:198:ARG:HA	2:3:212:ARG:O	2.19	0.42
3:4:375:ASP:HA	3:4:377:ASN:O	2.19	0.42
5:6:510:SER:HA	5:6:513:ILE:CB	2.48	0.42
1:2:564:VAL:O	1:2:605:LEU:N	2.37	0.42
2:3:270:LEU:CA	4:5:510:THR:H	2.32	0.42
5:6:152:TYR:HA	5:6:266:SER:O	2.19	0.42
5:6:288:LEU:H	5:6:399:GLY:HA3	1.84	0.42
6:7:334:HIS:CB	6:7:377:GLU:HA	2.50	0.42
2:3:536:PRO:HA	2:3:537:ASP:HA	1.55	0.42
2:3:669:PRO:HA	2:3:719:LYS:C	2.39	0.42
4:5:401:PRO:HA	4:5:402:ASP:C	2.38	0.42
5:6:810:ILE:O	5:6:813:ALA:HB3	2.19	0.42
1:2:220:ASP:O	1:2:223:GLY:O	2.38	0.42
2:3:38:TYR:O	2:3:41:SER:N	2.52	0.42
3:4:329:LYS:HA	3:4:433:ILE:O	2.19	0.42
3:4:880:SER:CB	3:4:926:SER:H	2.32	0.42
3:4:917:ILE:O	3:4:926:SER:O	2.38	0.42
3:4:917:ILE:CB	3:4:928:ARG:H	2.32	0.42
5:6:559:THR:N	5:6:564:LYS:HA	2.35	0.42
4:5:752:LEU:O	4:5:755:LEU:N	2.51	0.42
3:4:598:ALA:HB2	3:4:640:SER:O	2.19	0.42
4:5:708:LEU:O	4:5:712:ARG:CB	2.66	0.42
5:6:336:PRO:C	5:6:338:CYS:H	2.21	0.42
1:2:497:ILE:C	1:2:500:SER:H	2.21	0.42
3:4:408:ASP:CB	3:4:409:GLY:HA2	2.50	0.42
3:4:594:LYS:C	3:4:596:SER:N	2.73	0.42
5:6:600:GLY:HA2	5:6:640:GLU:CB	2.50	0.42
6:7:395:SER:C	6:7:397:VAL:N	2.73	0.42
7:C:199:PHE:O	7:C:228:LEU:HA	2.20	0.42
1:2:254:ALA:O	1:2:257:ALA:N	2.53	0.42
3:4:339:ILE:O	3:4:393:ASP:HA	2.19	0.42
4:5:760:THR:O	4:5:764:ARG:N	2.43	0.42
5:6:399:GLY:O	5:6:455:LEU:O	2.38	0.42
6:7:357:PRO:CA	6:7:374:THR:HA	2.44	0.42
6:7:703:ARG:C	6:7:705:ALA:H	2.23	0.42
1:2:425:GLU:O	1:2:456:ILE:HA	2.20	0.42
3:4:377:ASN:CB	3:4:378:GLU:CA	2.96	0.42
4:5:62:THR:HA	4:5:138:ILE:O	2.19	0.42
2:3:534:ALA:HA	4:5:758:HIS:O	2.20	0.42
5:6:603:SER:N	5:6:604:SER:HA	2.23	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:455:ASN:O	6:7:595:ASP:N	2.53	0.42
6:7:465:ALA:O	6:7:466:LYS:C	2.58	0.42
7:C:536:SER:O	7:C:539:VAL:N	2.53	0.42
1:2:219:THR:CB	7:C:84:GLU:CB	2.98	0.42
1:2:370:LYS:C	1:2:372:PRO:N	2.74	0.42
2:3:314:LEU:C	4:5:459:THR:HA	2.40	0.42
3:4:256:ASP:O	3:4:259:HIS:N	2.53	0.42
5:6:386:VAL:C	5:6:388:ARG:H	2.22	0.42
5:6:797:VAL:C	5:6:799:GLN:N	2.73	0.42
6:7:525:GLU:O	6:7:528:LYS:N	2.41	0.42
1:2:223:GLY:N	7:C:86:ASP:C	2.73	0.42
1:2:505:ILE:C	1:2:507:GLY:H	2.23	0.41
1:2:552:ILE:O	1:2:555:TYR:N	2.53	0.41
2:3:100:LEU:H	2:3:159:GLY:H	1.67	0.41
2:3:191:LEU:N	2:3:455:ARG:C	2.73	0.41
2:3:201:HIS:HA	2:3:243:THR:HA	2.02	0.41
6:7:259:ALA:HA	6:7:269:VAL:O	2.20	0.41
1:2:332:PRO:O	1:2:382:TYR:O	2.38	0.41
5:6:309:PHE:CB	5:6:346:LEU:HA	2.50	0.41
5:6:337:SER:C	5:6:339:GLU:H	2.24	0.41
1:2:317:LEU:HA	1:2:429:ILE:HA	2.02	0.41
1:2:324:VAL:CB	1:2:420:PRO:HA	2.50	0.41
2:3:234:GLU:HA	2:3:240:LYS:HA	2.01	0.41
3:4:484:GLU:O	3:4:487:GLN:N	2.52	0.41
1:2:244:VAL:O	1:2:297:ILE:C	2.58	0.41
3:4:447:ASN:C	3:4:449:ARG:H	2.23	0.41
3:4:855:SER:CA	3:4:857:ILE:N	2.83	0.41
6:7:247:ARG:O	6:7:508:LEU:O	2.38	0.41
6:7:483:THR:O	6:7:524:ASP:N	2.53	0.41
2:3:338:ALA:HB3	2:3:339:ARG:C	2.41	0.41
6:7:499:LYS:CA	6:7:506:MET:H	2.31	0.41
1:2:207:ILE:O	1:2:208:ALA:C	2.59	0.41
2:3:323:GLY:HA3	2:3:324:ASN:HA	1.55	0.41
3:4:713:ASP:O	3:4:716:ASN:N	2.54	0.41
4:5:40:LEU:O	4:5:43:GLN:N	2.54	0.41
4:5:665:LYS:C	4:5:668:LEU:H	2.23	0.41
2:3:688:ASN:HA	6:7:604:PRO:CB	2.50	0.41
7:C:348:SER:O	7:C:352:LYS:N	2.54	0.41
1:2:290:HIS:C	1:2:292:GLU:H	2.23	0.41
3:4:445:ARG:HA	3:4:453:LEU:HA	2.03	0.41
4:5:86:ILE:O	4:5:89:LEU:N	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:518:ASN:H	6:7:560:ARG:C	2.24	0.41
7:C:597:ILE:O	7:C:601:LYS:HA	2.20	0.41
1:2:787:SER:O	1:2:790:TYR:N	2.53	0.41
2:3:411:PRO:C	2:3:413:THR:N	2.73	0.41
4:5:754:ALA:O	4:5:758:HIS:N	2.51	0.41
5:6:301:ARG:N	5:6:356:TRP:O	2.45	0.41
5:6:543:VAL:O	5:6:544:LYS:C	2.58	0.41
7:C:509:LEU:O	7:C:512:LYS:N	2.54	0.41
7:C:89:LEU:O	7:C:90:GLU:C	2.59	0.41
2:3:448:THR:CB	6:7:363:PHE:H	2.33	0.41
5:6:766:THR:C	5:6:768:GLU:O	2.59	0.41
5:6:763:PRO:HA	5:6:817:ASP:CB	2.51	0.41
1:2:500:SER:HA	1:2:757:PRO:CB	2.50	0.41
1:2:802:SER:HA	1:2:803:PHE:HA	1.80	0.41
3:4:608:ASP:C	3:4:610:ASP:N	2.74	0.41
3:4:729:LEU:HA	3:4:730:GLU:HA	1.68	0.41
4:5:415:LEU:HA	4:5:523:ALA:O	2.20	0.41
5:6:637:CYS:HA	5:6:679:LEU:O	2.20	0.41
5:6:751:LEU:O	5:6:752:ARG:C	2.58	0.41
6:7:212:ALA:O	6:7:216:ARG:N	2.46	0.41
7:C:197:THR:O	7:C:230:PHE:HA	2.21	0.41
1:2:425:GLU:N	1:2:457:LYS:O	2.38	0.41
2:3:449:ASP:CB	6:7:366:LEU:CB	2.99	0.41
3:4:771:VAL:O	3:4:772:ARG:C	2.59	0.41
5:6:173:GLN:O	5:6:176:ARG:N	2.54	0.41
6:7:208:SER:CB	6:7:209:GLN:HA	2.51	0.41
3:4:335:SER:HA	3:4:396:VAL:O	2.22	0.40
3:4:766:ALA:O	3:4:767:LYS:C	2.59	0.40
3:4:811:MET:C	3:4:813:LEU:H	2.24	0.40
4:5:237:GLY:HA2	4:5:238:PRO:O	2.21	0.40
6:7:249:SER:CA	6:7:507:ILE:CA	2.92	0.40
2:3:474:GLU:O	2:3:477:LYS:N	2.54	0.40
2:3:735:PHE:HA	2:3:738:LEU:O	2.21	0.40
3:4:621:LEU:O	3:4:624:SER:N	2.54	0.40
5:6:170:ILE:O	5:6:171:SER:C	2.58	0.40
5:6:731:ILE:O	5:6:732:VAL:C	2.58	0.40
1:2:602:GLY:O	1:2:644:CYS:HA	2.22	0.40
2:3:235:ASP:N	2:3:239:ASN:O	2.54	0.40
2:3:539:LEU:O	2:3:542:ARG:N	2.53	0.40
5:6:512:GLU:O	5:6:513:ILE:C	2.60	0.40
7:C:520:LEU:O	7:C:523:LEU:N	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:96:ILE:O	2:3:155:LEU:HA	2.22	0.40
3:4:910:LEU:O	3:4:916:VAL:N	2.55	0.40
4:5:415:LEU:CB	4:5:523:ALA:HB3	2.50	0.40
5:6:512:GLU:C	5:6:514:ASN:N	2.73	0.40
2:3:533:ILE:O	2:3:534:ALA:HB3	2.21	0.40
3:4:292:ASP:N	3:4:293:LEU:HA	2.35	0.40
3:4:488:ASN:C	3:4:490:VAL:H	2.23	0.40
3:4:778:ARG:HA	3:4:793:ALA:HB3	2.02	0.40
7:C:41:ASP:CB	7:C:246:THR:HA	2.51	0.40
7:C:363:LEU:O	7:C:367:TRP:N	2.51	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	2	583/868 (67%)	503 (86%)	69 (12%)	11 (2%)	10	52
2	3	589/971 (61%)	516 (88%)	65 (11%)	8 (1%)	14	58
3	4	706/933 (76%)	603 (85%)	95 (14%)	8 (1%)	17	63
4	5	614/775 (79%)	564 (92%)	45 (7%)	5 (1%)	24	69
5	6	634/1017 (62%)	539 (85%)	80 (13%)	15 (2%)	7	47
6	7	612/845 (72%)	542 (89%)	62 (10%)	8 (1%)	15	60
7	C	419/604 (69%)	353 (84%)	65 (16%)	1 (0%)	52	86
All	All	4157/6013 (69%)	3620 (87%)	481 (12%)	56 (1%)	20	60

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	305	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	334	LEU
2	3	198	ARG
3	4	179	ILE
3	4	490	VAL
3	4	609	VAL
4	5	267	VAL
4	5	596	ILE
5	6	510	SER
5	6	513	ILE
5	6	578	SER
5	6	605	ALA
6	7	26	VAL
6	7	464	VAL
6	7	544	GLN
1	2	297	ILE
1	2	533	ILE
1	2	548	ALA
2	3	389	VAL
3	4	419	VAL
3	4	857	ILE
4	5	177	THR
5	6	321	VAL
5	6	402	ILE
5	6	580	SER
6	7	502	VAL
7	C	221	SER
1	2	585	ILE
2	3	230	ILE
4	5	410	ILE
5	6	555	VAL
5	6	579	THR
5	6	703	ALA
6	7	373	GLU
4	5	460	ARG
5	6	781	ARG
6	7	371	LEU
1	2	256	LEU
1	2	550	SER
2	3	158	LYS
2	3	440	VAL
3	4	773	ALA
5	6	556	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	6	653	HIS
1	2	265	GLU
1	2	291	SER
3	4	463	VAL
5	6	533	ILE
6	7	248	VAL
1	2	840	VAL
3	4	526	ILE
2	3	326	VAL
2	3	20	VAL
2	3	533	ILE
5	6	503	VAL
6	7	708	VAL

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.