



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:02 AM UTC

PDB ID : 8Y08 / pdb_00008y08
Title : Crystal structure of LbCas12a in complex with crRNA and 14nt target DNA
Authors : Lin, X.; Chen, J.; Liu, L.
Deposited on : 2024-01-22
Resolution : 3.64 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

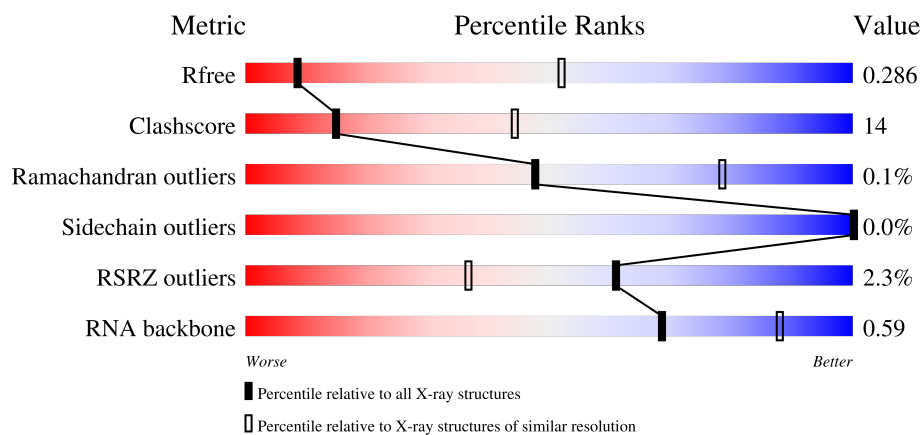
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.64 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1132 (3.76-3.52)
Clashscore	190562	1014 (3.74-3.54)
Ramachandran outliers	187476	1123 (3.76-3.52)
Sidechain outliers	187428	1121 (3.76-3.52)
RSRZ outliers	180081	1130 (3.76-3.52)
RNA backbone	3983	1026 (4.22-3.06)

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

Mol	Chain	Length	Quality of chain
1	A	1228	2% 67% 32%
1	E	1228	2% 71% 28%
2	B	40	38% 48% 12%
2	F	40	35% 50% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	23	
3	G	23	
4	D	11	
4	H	11	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	LI	A	1301	-	-	-	X
5	LI	A	1302	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 22796 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 LbCas12a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1223	Total	C	N	O	S	0	0	0
			9964	6412	1623	1900	29			
1	E	1223	Total	C	N	O	S	0	0	0
			9964	6412	1623	1900	29			

- Molecule 2 is a RNA chain called RNA (35-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	35	Total	C	N	O	P	0	0	0
			739	333	131	241	34			
2	F	35	Total	C	N	O	P	0	0	0
			739	333	131	241	34			

- Molecule 3 is a DNA chain called DNA (5'-D(P*CP*TP*TP*TP*AP*CP*TP*GP*GP*AP*TP*GP*CP*GP*TP*AP*AP*AP*GP*GP*AP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	23	Total	C	N	O	P	0	0	0
			476	226	89	138	23			
3	G	23	Total	C	N	O	P	0	0	0
			476	226	89	138	23			

- Molecule 4 is a DNA chain called DNA (5'-D(*CP*GP*TP*CP*CP*TP*TP*TP*AP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	11	Total	C	N	O	P	0	0	0
			217	107	31	69	10			
4	H	11	Total	C	N	O	P	0	0	0
			217	107	31	69	10			

- Molecule 5 is LITHIUM ION (CCD ID: LI) (formula: Li).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total 2	Li 2	0	0
5	B	1	Total 1	Li 1	0	0

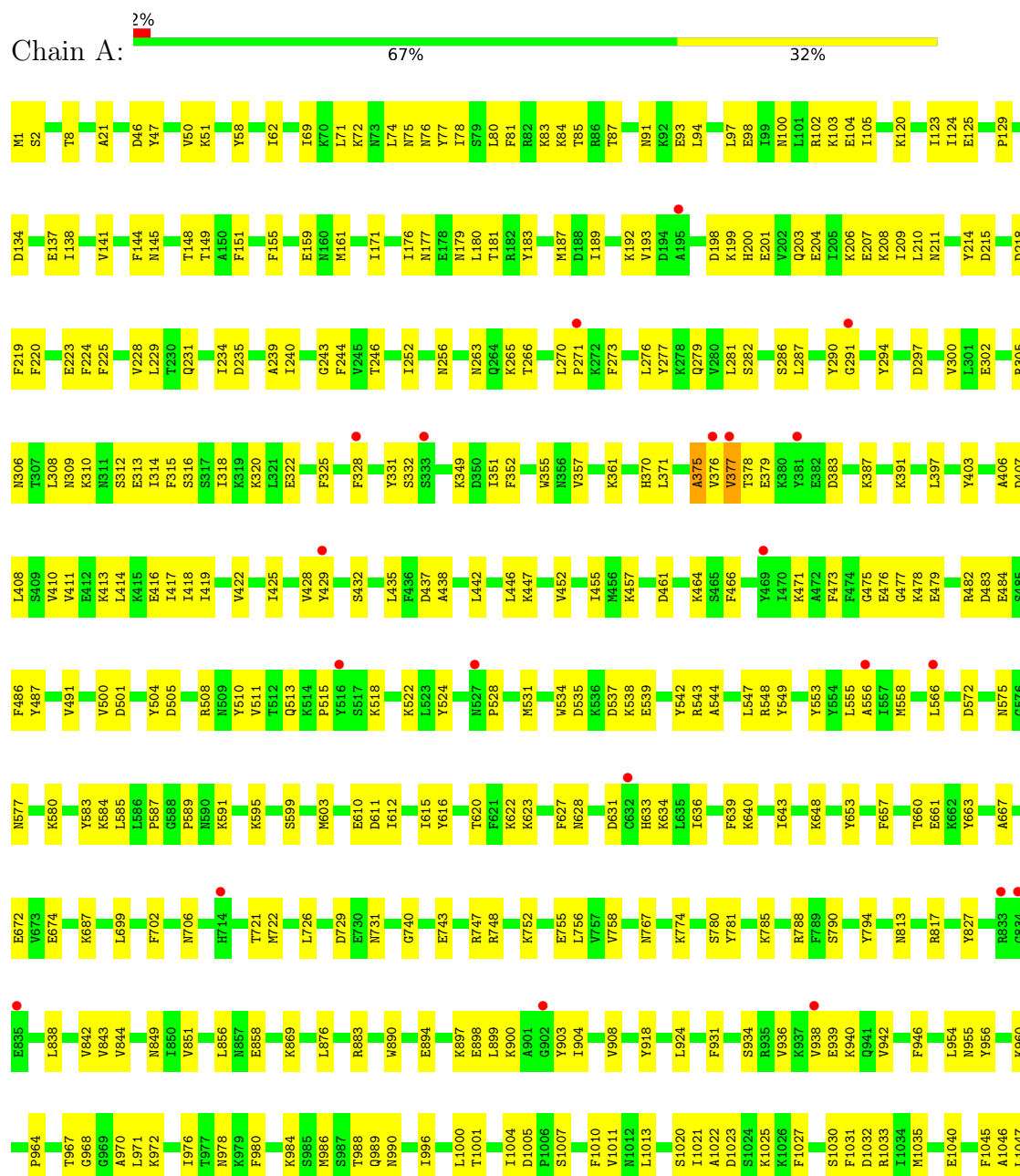
- Molecule 6 is water.

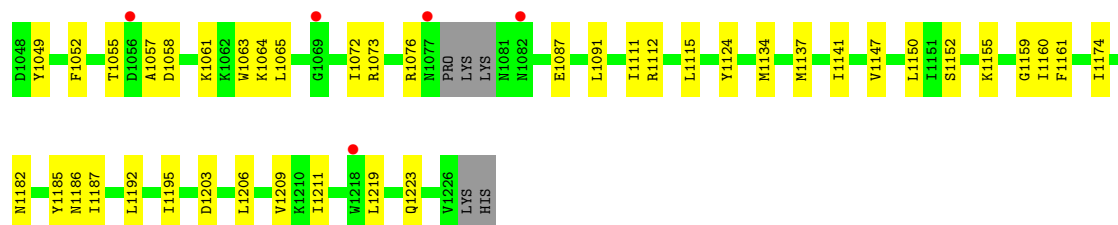
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	1	Total 1	O 1	0	0

3 Residue-property plots

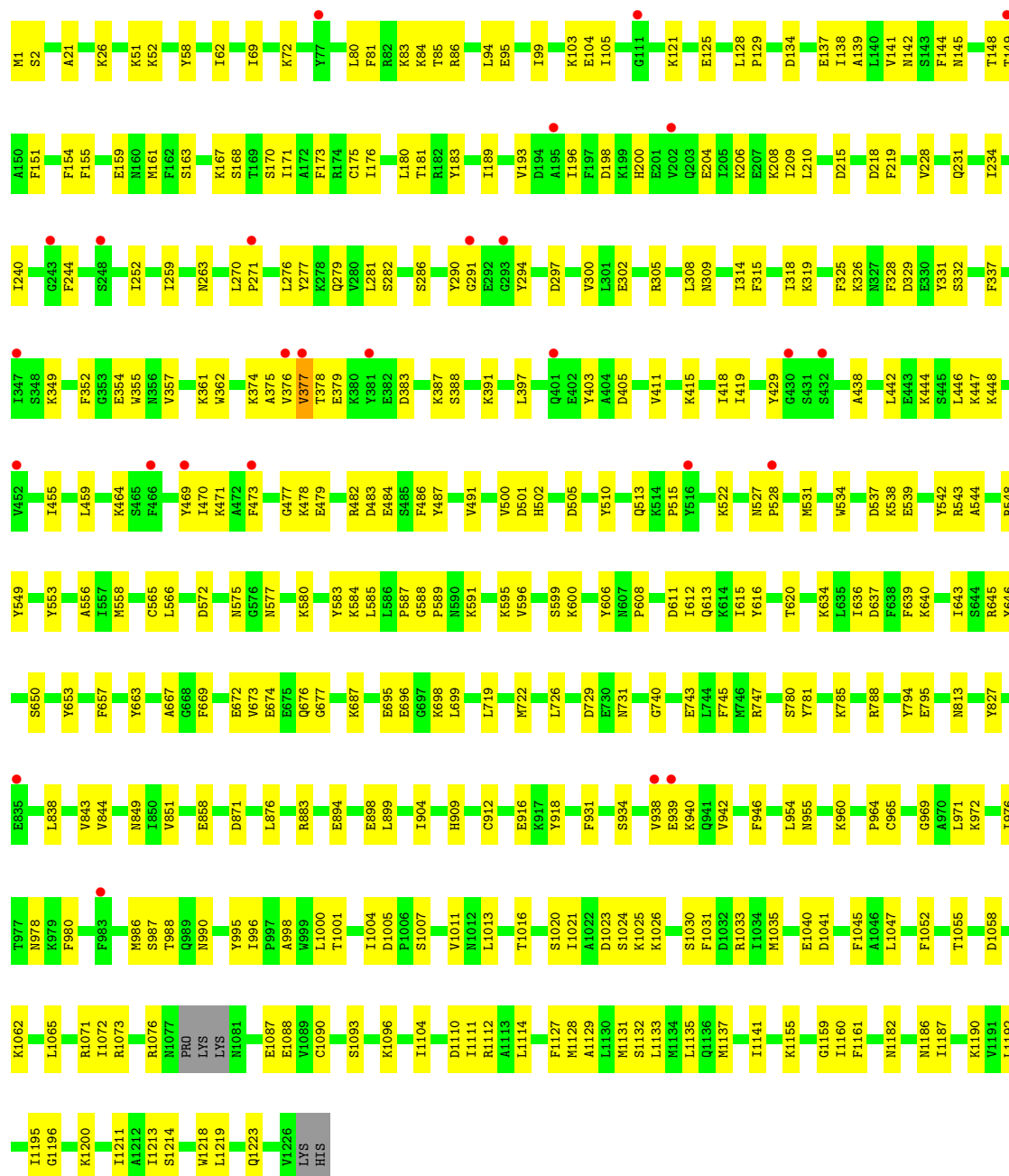
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: LbCas12a

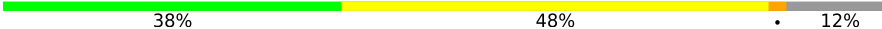




• Molecule 1: LbCas12a

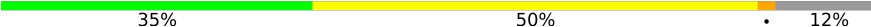


• Molecule 2: RNA (35-MER)

Chain B:  38% 48% 12%



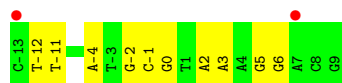
- Molecule 2: RNA (35-MER)

Chain F:  35% 50% 12%



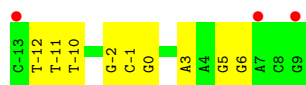
- Molecule 3: DNA (5'-D(P*CP*TP*TP*TP*AP*CP*TP*GP*GP*AP*TP*GP*CP*GP*TP*AP*AP*AP*GP*GP*AP*CP*G)-3')

Chain C:  9% 57% 43%



- Molecule 3: DNA (5'-D(P*CP*TP*TP*TP*AP*CP*TP*GP*GP*AP*TP*GP*CP*GP*TP*AP*AP*AP*GP*GP*AP*CP*G)-3')

Chain G:  13% 61% 39%



- Molecule 4: DNA (5'-D(*CP*GP*TP*CP*CP*TP*TP*TP*AP*TP*T)-3')

Chain D:  55% 45%



- Molecule 4: DNA (5'-D(*CP*GP*TP*CP*CP*TP*TP*TP*AP*TP*T)-3')

Chain H:  9% 64% 36%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.39Å 142.29Å 208.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.07 – 3.64 26.07 – 3.64	Depositor EDS
% Data completeness (in resolution range)	90.5 (26.07-3.64) 90.5 (26.07-3.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.252 , 0.285 0.252 , 0.286	Depositor DCC
R_{free} test set	1885 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 9.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	22796	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.88 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0752e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
LI

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.18	0/10174	0.43	2/13698 (0.0%)
1	E	0.17	0/10174	0.41	0/13698
2	B	0.12	0/826	0.30	0/1284
2	F	0.12	0/826	0.29	0/1284
3	C	0.19	0/534	0.38	0/823
3	G	0.19	0/534	0.38	0/823
4	D	0.25	0/240	0.50	0/368
4	H	0.22	0/240	0.48	0/368
All	All	0.17	0/23548	0.41	2/32346 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	ALA	CA-C-N	5.00	130.98	121.97
1	A	375	ALA	C-N-CA	5.00	130.98	121.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	9964	0	9743	321	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	9964	0	9743	256	1
2	B	739	0	377	16	0
2	F	739	0	377	15	0
3	C	476	0	260	10	0
3	G	476	0	260	12	0
4	D	217	0	129	5	0
4	H	217	0	129	4	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
6	E	1	0	0	0	0
All	All	22796	0	21018	601	1

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 14.

All (601) 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:1141:ILE:HB	1:A:1147:VAL:HG21	1.56	0.85
1:E:538:LYS:NZ	3:G:3:DA:N7	2.26	0.83
1:A:538:LYS:NZ	3:C:3:DA:N7	2.26	0.82
1:A:522:LYS:HE3	1:A:743:GLU:HG2	1.60	0.81
1:E:636:ILE:HD13	1:E:663:TYR:HD2	1.46	0.80
1:A:595:LYS:O	1:A:599:SER:OG	1.99	0.79
1:E:1190:LYS:HE3	1:E:1213:ILE:HG21	1.64	0.79
1:E:1016:THR:HG1	1:E:1132:SER:HG	1.28	0.79
1:A:183:TYR:OH	1:A:219:PHE:O	1.99	0.78
1:A:208:LYS:HG3	1:A:252:ILE:HD12	1.65	0.78
1:E:479:GLU:OE2	1:E:482:ARG:NH1	2.16	0.77
1:E:522:LYS:HE3	1:E:743:GLU:HG2	1.66	0.77
1:A:636:ILE:HD13	1:A:663:TYR:HD2	1.50	0.77
1:E:314:ILE:HD13	1:E:500:VAL:HG12	1.66	0.76
1:E:183:TYR:OH	1:E:219:PHE:O	2.02	0.76
1:E:955:ASN:HD21	1:E:980:PHE:H	1.32	0.76
1:E:308:LEU:O	1:E:429:TYR:OH	2.04	0.75
1:A:361:LYS:NZ	1:A:403:TYR:O	2.20	0.75
1:E:1033:ARG:NH2	1:E:1035:MET:SD	2.58	0.75
1:A:986:MET:HE1	1:A:990:ASN:HD22	1.52	0.75
1:A:813:ASN:OD1	1:A:978:ASN:ND2	2.20	0.74
1:A:897:LYS:NZ	1:A:898:GLU:OE2	2.19	0.74
1:A:308:LEU:O	1:A:429:TYR:OH	2.05	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:GLU:OE2	1:A:580:LYS:NZ	2.20	0.74
1:A:87:THR:O	1:A:91:ASN:N	2.21	0.73
1:E:537:ASP:OD2	1:E:584:LYS:NZ	2.21	0.73
1:E:80:LEU:HB3	1:E:94:LEU:HD13	1.70	0.73
1:A:1073:ARG:NH2	1:A:1087:GLU:OE1	2.23	0.72
1:E:376:VAL:HG13	1:E:377:VAL:HG22	1.72	0.71
1:A:479:GLU:OE2	1:A:482:ARG:NH1	2.23	0.71
1:E:305:ARG:O	1:E:309:ASN:ND2	2.22	0.71
1:E:596:VAL:HG11	1:E:646:TYR:HE1	1.55	0.70
1:E:813:ASN:OD1	1:E:978:ASN:ND2	2.21	0.70
1:A:464:LYS:NZ	1:A:501:ASP:OD2	2.25	0.70
1:A:211:ASN:O	1:A:211:ASN:ND2	2.25	0.69
1:A:752:LYS:HB3	1:A:755:GLU:HG3	1.75	0.69
1:A:203:GLN:O	1:A:207:GLU:N	2.21	0.69
1:A:464:LYS:NZ	2:B:14:C:OP1	2.26	0.69
1:A:595:LYS:NZ	4:D:-2:DT:O2	2.26	0.69
1:A:1033:ARG:NH2	1:A:1035:MET:SD	2.66	0.68
1:E:464:LYS:NZ	1:E:501:ASP:OD2	2.24	0.68
1:A:1020:SER:OG	1:A:1023:ASP:OD1	2.10	0.68
1:E:584:LYS:HB3	1:E:653:TYR:HE1	1.57	0.68
1:E:1:MET:HE3	1:E:2:SER:HA	1.76	0.68
1:E:200:HIS:O	1:E:204:GLU:N	2.21	0.68
1:E:447:LYS:HB3	1:E:515:PRO:HG3	1.76	0.68
1:E:464:LYS:NZ	2:F:14:C:OP1	2.26	0.68
1:A:1045:PHE:HB2	1:A:1065:LEU:HB2	1.75	0.68
1:A:102:ARG:NH1	1:A:177:ASN:OD1	2.26	0.68
1:E:326:LYS:HA	1:E:415:LYS:HG3	1.76	0.68
1:A:265:LYS:HG2	1:A:266:THR:HG23	1.76	0.67
1:A:729:ASP:OD1	1:A:731:ASN:ND2	2.26	0.67
1:A:75:ASN:HD21	1:A:223:GLU:HG2	1.58	0.67
1:A:1182:ASN:O	1:A:1186:ASN:ND2	2.28	0.66
1:E:729:ASP:OD1	1:E:731:ASN:ND2	2.28	0.66
1:A:83:LYS:NZ	1:A:85:THR:O	2.27	0.66
1:E:305:ARG:HH21	1:E:438:ALA:HA	1.61	0.66
1:A:1058:ASP:OD1	1:A:1223:GLN:NE2	2.21	0.66
1:E:539:GLU:OE2	1:E:580:LYS:NZ	2.27	0.66
1:A:305:ARG:O	1:A:309:ASN:ND2	2.26	0.66
1:E:876:LEU:HD23	1:E:899:LEU:HG	1.78	0.66
1:E:1155:LYS:HB3	1:E:1159:GLY:HA2	1.76	0.66
1:E:387:LYS:HE3	1:E:391:LYS:HE2	1.78	0.65
1:A:148:THR:OG1	4:D:-4:DT:OP1	2.14	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ASP:OD1	1:A:510:TYR:OH	2.13	0.65
1:E:1016:THR:OG1	1:E:1132:SER:OG	2.12	0.65
1:A:537:ASP:OD2	1:A:584:LYS:NZ	2.29	0.65
1:A:1141:ILE:HB	1:A:1147:VAL:CG2	2.24	0.65
1:A:486:PHE:HD2	1:A:487:TYR:HD2	1.43	0.65
1:A:934:SER:HB3	1:A:938:VAL:HG22	1.79	0.65
1:E:129:PRO:HA	1:E:138:ILE:HD11	1.80	0.64
2:F:9:U:H2'	2:F:10:A:H8	1.62	0.64
1:A:447:LYS:HB3	1:A:515:PRO:HG3	1.80	0.64
1:A:231:GLN:HB2	1:A:279:GLN:HG2	1.79	0.64
1:E:176:ILE:O	1:E:180:LEU:HB2	1.98	0.64
1:E:279:GLN:HG3	1:E:282:SER:HB3	1.80	0.64
1:A:218:ASP:HB3	1:A:224:PHE:CE1	2.33	0.63
1:E:934:SER:HB3	1:E:938:VAL:HG22	1.79	0.63
1:A:1155:LYS:HB3	1:A:1159:GLY:HA2	1.79	0.63
1:E:286:SER:OG	3:G:-12:DT:OP1	2.15	0.62
1:A:209:ILE:HG12	1:A:244:PHE:CE1	2.34	0.62
1:A:572:ASP:OD1	1:A:575:ASN:N	2.31	0.62
1:A:663:TYR:OH	1:A:672:GLU:OE2	2.09	0.62
1:E:206:LYS:HA	1:E:210:LEU:HB2	1.81	0.62
1:E:297:ASP:OD1	1:E:510:TYR:OH	2.16	0.62
1:E:996:ILE:HD11	1:E:1187:ILE:HG23	1.80	0.62
1:A:198:ASP:OD1	1:A:200:HIS:N	2.32	0.62
1:A:176:ILE:O	1:A:180:LEU:HB2	1.99	0.62
1:E:572:ASP:OD1	1:E:575:ASN:N	2.31	0.62
1:E:1192:LEU:HD23	1:E:1195:ILE:HD12	1.82	0.62
1:A:410:VAL:HG12	1:A:414:LEU:HD23	1.82	0.61
1:A:375:ALA:O	1:A:376:VAL:HG12	2.01	0.61
1:E:585:LEU:HG	1:E:587:PRO:HD3	1.81	0.61
1:E:645:ARG:HG3	1:E:645:ARG:HH21	1.66	0.61
2:B:9:U:H2'	2:B:10:A:H8	1.65	0.60
1:E:486:PHE:HD2	1:E:487:TYR:HD2	1.48	0.60
1:E:987:SER:OG	1:E:988:THR:N	2.33	0.60
1:E:1000:LEU:HD13	1:E:1011:VAL:HG11	1.83	0.60
1:A:428:VAL:O	1:A:432:SER:OG	2.18	0.60
1:A:531:MET:HG3	1:A:544:ALA:HB3	1.83	0.60
1:A:611:ASP:O	1:A:615:ILE:HG12	2.00	0.60
1:A:1027:PHE:O	1:A:1030:SER:OG	2.20	0.60
1:E:1058:ASP:OD1	1:E:1223:GLN:NE2	2.31	0.60
1:A:263:ASN:HD21	1:A:270:LEU:H	1.47	0.60
1:A:305:ARG:HH21	1:A:438:ALA:HA	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:LEU:HD21	1:A:452:VAL:HG21	1.83	0.59
1:A:290:TYR:HD2	1:A:291:GLY:H	1.50	0.59
1:E:667:ALA:HB2	4:H:1:DT:H2''	1.83	0.59
1:A:813:ASN:ND2	1:A:989:GLN:HG2	2.17	0.59
3:C:-12:DT:H2'	3:C:-11:DT:C6	2.38	0.59
1:E:26:LYS:HD2	1:E:695:GLU:HG3	1.84	0.59
1:E:302:GLU:HA	1:E:305:ARG:HD3	1.84	0.59
1:A:219:PHE:CD1	1:A:240:ILE:HD11	2.38	0.58
1:A:328:PHE:CE2	1:A:397:LEU:HD11	2.38	0.58
1:E:374:LYS:H	1:E:374:LYS:HD2	1.68	0.58
1:A:1031:PHE:O	1:A:1112:ARG:NH1	2.36	0.58
1:A:1031:PHE:CE2	1:A:1047:LEU:HD23	2.38	0.58
2:F:9:U:H2'	2:F:10:A:C8	2.38	0.58
1:A:955:ASN:HD21	1:A:980:PHE:H	1.51	0.58
1:A:206:LYS:NZ	1:A:215:ASP:OD1	2.36	0.58
1:A:209:ILE:HG12	1:A:244:PHE:HE1	1.69	0.58
1:A:722:MET:HE1	1:A:960:LYS:HA	1.85	0.57
1:A:375:ALA:HB1	1:A:378:THR:OG1	2.05	0.57
1:A:548:ARG:HD3	1:A:553:TYR:CE2	2.40	0.57
1:A:667:ALA:HB2	4:D:1:DT:H2''	1.86	0.57
2:B:9:U:H2'	2:B:10:A:C8	2.39	0.57
1:E:375:ALA:HB1	1:E:378:THR:OG1	2.03	0.57
1:A:781:TYR:OH	2:B:-19:A:N1	2.34	0.57
1:E:290:TYR:HD2	1:E:291:GLY:H	1.52	0.57
3:G:-12:DT:H2'	3:G:-11:DT:C6	2.40	0.57
1:E:81:PHE:HZ	1:E:181:THR:HG23	1.70	0.57
1:E:482:ARG:O	1:E:484:GLU:N	2.37	0.57
3:G:-2:DG:H2'	3:G:-1:DC:C6	2.40	0.57
1:A:785:LYS:HD2	2:B:-20:A:H5''	1.85	0.57
1:E:745:PHE:HB2	1:E:795:GLU:HB2	1.87	0.56
1:A:623:LYS:HA	1:A:627:PHE:HB2	1.86	0.56
1:A:1052:PHE:HB2	1:A:1055:THR:HG21	1.87	0.56
1:A:279:GLN:HG3	1:A:282:SER:HB3	1.87	0.56
1:A:856:LEU:O	1:A:903:TYR:OH	2.21	0.56
1:E:780:SER:O	1:E:780:SER:OG	2.22	0.56
1:A:286:SER:OG	3:C:-12:DT:OP1	2.19	0.56
1:E:290:TYR:HE1	3:G:-12:DT:H1'	1.70	0.56
1:A:256:ASN:OD1	1:A:273:PHE:N	2.34	0.56
1:E:487:TYR:O	1:E:491:VAL:HG23	2.06	0.56
1:A:482:ARG:O	1:A:484:GLU:N	2.38	0.56
1:A:996:ILE:HD11	1:A:1187:ILE:HG23	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1005:ASP:HB2	1:E:1137:MET:HE1	1.86	0.56
1:E:1011:VAL:HG11	1:E:1219:LEU:HD21	1.87	0.56
1:E:193:VAL:HG13	1:E:270:LEU:HD13	1.88	0.56
1:A:81:PHE:HZ	1:A:181:THR:HG23	1.71	0.56
1:A:628:ASN:HB3	1:A:631:ASP:HB2	1.88	0.55
1:E:375:ALA:O	1:E:376:VAL:HG12	2.06	0.55
1:E:672:GLU:O	1:E:676:GLN:HG2	2.06	0.55
1:A:322:GLU:OE1	1:A:422:VAL:HG21	2.06	0.55
3:C:-2:DG:H2'	3:C:-1:DC:C6	2.40	0.55
1:E:69:ILE:HD11	1:E:105:ILE:HG12	1.89	0.55
1:A:263:ASN:ND2	1:A:270:LEU:H	2.05	0.55
1:E:80:LEU:O	1:E:86:ARG:NH1	2.38	0.55
1:E:486:PHE:HD2	1:E:487:TYR:CD2	2.24	0.55
1:E:596:VAL:HG11	1:E:646:TYR:CE1	2.39	0.55
1:A:487:TYR:O	1:A:491:VAL:HG23	2.07	0.55
1:A:129:PRO:HA	1:A:138:ILE:HD11	1.87	0.54
1:A:300:VAL:HG21	1:A:510:TYR:CD2	2.42	0.54
1:A:325:PHE:CD1	1:A:418:ILE:HG13	2.42	0.54
1:A:785:LYS:HB2	2:B:-20:A:H5''	1.89	0.54
1:A:332:SER:N	1:A:483:ASP:OD1	2.34	0.54
1:E:1031:PHE:O	1:E:1112:ARG:NH1	2.29	0.54
1:A:325:PHE:O	1:A:328:PHE:HB2	2.06	0.54
1:A:1000:LEU:HD13	1:A:1011:VAL:HG11	1.90	0.54
1:A:1206:LEU:HA	1:A:1209:VAL:HG23	1.88	0.54
1:E:148:THR:OG1	4:H:-4:DT:OP1	2.21	0.54
1:A:774:LYS:NZ	2:B:-10:A:OP2	2.39	0.54
1:A:206:LYS:HA	1:A:210:LEU:HG	1.89	0.54
1:E:325:PHE:HE1	1:E:473:PHE:HE2	1.55	0.54
1:E:1045:PHE:HB2	1:E:1065:LEU:HB2	1.90	0.54
1:A:305:ARG:NH2	1:A:437:ASP:O	2.40	0.54
1:E:785:LYS:HD2	2:F:-20:A:H5''	1.88	0.54
1:A:290:TYR:HE1	3:C:-12:DT:H1'	1.72	0.54
1:E:615:ILE:HG23	1:E:620:THR:OG1	2.08	0.54
1:A:309:ASN:O	1:A:312:SER:OG	2.26	0.53
1:E:290:TYR:HD2	1:E:291:GLY:N	2.06	0.53
1:E:376:VAL:O	1:E:377:VAL:HG13	2.08	0.53
1:A:575:ASN:O	1:A:577:ASN:ND2	2.41	0.53
1:A:290:TYR:HD2	1:A:291:GLY:N	2.06	0.53
1:A:1032:ASP:C	1:A:1112:ARG:HH12	2.16	0.53
1:E:209:ILE:HG12	1:E:244:PHE:HE1	1.71	0.53
1:A:328:PHE:HD2	1:A:411:VAL:HG23	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:VAL:HG23	1:A:377:VAL:O	2.08	0.53
1:A:1141:ILE:HD12	1:A:1147:VAL:HG21	1.90	0.53
1:E:785:LYS:HB2	2:F:-20:A:H5''	1.90	0.53
1:A:198:ASP:HB3	1:A:201:GLU:HB2	1.91	0.53
1:A:1057:ALA:HB1	1:A:1219:LEU:HD12	1.91	0.53
1:E:1026:LYS:O	1:E:1030:SER:OG	2.26	0.53
1:A:956:TYR:OH	1:A:970:ALA:O	2.22	0.53
1:E:740:GLY:O	3:G:0:DG:H2''	2.09	0.53
1:A:584:LYS:HB3	1:A:653:TYR:HE1	1.74	0.53
1:A:1203:ASP:HA	1:A:1206:LEU:CD1	2.40	0.52
1:E:612:ILE:HD11	1:E:634:LYS:HG2	1.91	0.52
1:E:1004:ILE:HG13	1:E:1011:VAL:HG12	1.91	0.52
1:A:306:ASN:O	1:A:312:SER:HB3	2.10	0.52
1:A:349:LYS:HD3	1:A:355:TRP:HE1	1.73	0.52
1:A:432:SER:HB3	1:A:455:ILE:HG23	1.92	0.52
1:A:904:ILE:HG22	1:A:908:VAL:HG23	1.90	0.52
1:E:584:LYS:HB3	1:E:653:TYR:CE1	2.42	0.52
1:E:1021:ILE:O	1:E:1025:LYS:HG3	2.09	0.52
1:A:817:ARG:HB3	1:A:1206:LEU:HD23	1.92	0.52
1:E:328:PHE:CE2	1:E:397:LEU:HD11	2.44	0.52
1:A:838:LEU:HD21	1:A:939:GLU:OE1	2.09	0.52
1:E:1182:ASN:O	1:E:1186:ASN:ND2	2.42	0.52
1:E:210:LEU:HD21	1:E:240:ILE:HD11	1.90	0.52
1:E:556:ALA:HB1	1:E:699:LEU:HD11	1.91	0.52
1:E:209:ILE:HG12	1:E:244:PHE:CE1	2.45	0.51
1:E:105:ILE:HD11	1:E:176:ILE:HD11	1.91	0.51
1:A:639:PHE:O	1:A:643:ILE:HG13	2.10	0.51
1:E:176:ILE:HA	1:E:180:LEU:HD23	1.91	0.51
1:E:361:LYS:NZ	1:E:403:TYR:O	2.44	0.51
1:E:1001:THR:O	1:E:1186:ASN:ND2	2.43	0.51
1:A:93:GLU:O	1:A:97:LEU:HD12	2.10	0.51
1:A:938:VAL:HG12	1:A:940:LYS:H	1.74	0.51
2:B:11:A:H2'	2:B:12:A:C8	2.45	0.51
1:E:611:ASP:O	1:E:615:ILE:HG12	2.09	0.51
1:E:1104:ILE:HG23	1:E:1114:LEU:HG	1.91	0.51
1:A:328:PHE:HE2	1:A:397:LEU:HD11	1.75	0.51
1:A:780:SER:O	1:A:780:SER:OG	2.25	0.51
1:E:898:GLU:HG2	2:F:-15:C:H4'	1.93	0.51
1:E:349:LYS:HD3	1:E:355:TRP:HE1	1.76	0.51
1:A:1001:THR:O	1:A:1186:ASN:ND2	2.44	0.51
1:A:1022:ALA:HA	1:A:1025:LYS:HD3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:MET:O	1:A:171:ILE:HG13	2.11	0.51
1:A:325:PHE:HA	1:A:328:PHE:CD1	2.46	0.51
1:A:486:PHE:HD2	1:A:487:TYR:CD2	2.26	0.51
1:A:361:LYS:HG3	1:A:403:TYR:HB3	1.92	0.50
1:E:1024:SER:HB3	1:E:1128:MET:HE3	1.92	0.50
2:F:-1:U:O2'	2:F:1:G:OP1	2.26	0.50
1:A:964:PRO:HA	1:A:970:ALA:H	1.76	0.50
1:A:1058:ASP:OD2	1:A:1063:TRP:NE1	2.44	0.50
1:E:198:ASP:OD1	1:E:200:HIS:N	2.34	0.50
1:E:231:GLN:N	1:E:279:GLN:OE1	2.38	0.50
1:A:612:ILE:HD11	1:A:634:LYS:HG2	1.93	0.50
1:A:316:SER:O	1:A:320:LYS:HG2	2.11	0.50
1:A:747:ARG:NH2	1:A:788:ARG:O	2.44	0.50
1:A:74:LEU:O	1:A:78:ILE:HG13	2.12	0.50
1:E:300:VAL:HG21	1:E:510:TYR:CD2	2.47	0.50
1:A:75:ASN:ND2	1:A:223:GLU:HG2	2.26	0.50
1:E:325:PHE:CE1	1:E:473:PHE:HE2	2.30	0.50
1:E:483:ASP:O	1:E:486:PHE:N	2.43	0.50
1:E:988:THR:HG23	1:E:995:TYR:O	2.12	0.50
1:A:1005:ASP:OD1	1:A:1007:SER:OG	2.23	0.49
1:A:189:ILE:HG23	1:A:271:PRO:HG2	1.94	0.49
1:E:405:ASP:OD2	1:E:405:ASP:N	2.43	0.49
1:E:99:ILE:HG22	1:E:103:LYS:HE3	1.93	0.49
1:E:144:PHE:CD2	1:E:151:PHE:HE1	2.30	0.49
1:E:1073:ARG:HH12	1:E:1076:ARG:NH2	2.09	0.49
1:E:121:LYS:H	4:H:-3:DT:P	2.35	0.49
1:E:1129:ALA:O	1:E:1133:LEU:HD12	2.11	0.49
1:A:87:THR:O	1:A:91:ASN:ND2	2.42	0.49
1:E:83:LYS:HG3	1:E:85:THR:H	1.77	0.49
1:E:645:ARG:HG3	1:E:645:ARG:NH2	2.27	0.49
1:A:8:THR:HG21	1:A:967:THR:HG23	1.93	0.49
1:A:464:LYS:HZ2	2:B:14:C:P	2.36	0.49
1:A:522:LYS:HD3	1:A:524:TYR:CZ	2.48	0.49
1:E:125:GLU:HG2	1:E:145:ASN:OD1	2.12	0.49
1:E:138:ILE:O	1:E:142:ASN:ND2	2.46	0.49
1:A:75:ASN:ND2	1:A:223:GLU:OE2	2.46	0.49
1:A:144:PHE:CD2	1:A:151:PHE:HE1	2.30	0.49
1:E:149:THR:OG1	1:E:528:PRO:HB2	2.13	0.49
1:E:548:ARG:HD3	1:E:553:TYR:CE2	2.48	0.49
1:A:310:LYS:HG3	1:A:315:PHE:CE2	2.48	0.49
1:A:331:TYR:CD2	1:A:486:PHE:HD1	2.30	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:LEU:H	1:A:408:LEU:HD23	1.78	0.49
1:A:1073:ARG:HH12	1:A:1076:ARG:NH2	2.11	0.49
1:E:1072:ILE:HD13	1:E:1141:ILE:HD11	1.95	0.48
1:A:69:ILE:HD11	1:A:71:LEU:HD11	1.96	0.48
1:E:175:CYS:O	1:E:180:LEU:HD23	2.13	0.48
1:A:47:TYR:CZ	1:A:51:LYS:HD2	2.48	0.48
1:A:556:ALA:HB1	1:A:699:LEU:HD11	1.96	0.48
1:E:332:SER:N	1:E:483:ASP:OD1	2.41	0.48
1:A:406:ALA:HB1	1:A:407:ASP:HA	1.95	0.48
1:A:510:TYR:O	1:A:513:GLN:HG2	2.14	0.48
1:E:1076:ARG:H	1:E:1076:ARG:HE	1.62	0.48
1:A:934:SER:HB3	1:A:938:VAL:CG2	2.44	0.48
1:E:189:ILE:HG23	1:E:271:PRO:HG2	1.96	0.48
1:E:747:ARG:NH2	1:E:788:ARG:O	2.46	0.48
1:E:1005:ASP:OD1	1:E:1007:SER:OG	2.22	0.48
1:A:352:PHE:HE2	1:A:357:VAL:HB	1.79	0.48
1:A:968:GLY:N	1:A:972:LYS:O	2.42	0.48
1:E:722:MET:HE1	1:E:960:LYS:HA	1.95	0.48
1:E:1041:ASP:OD1	1:E:1096:LYS:NZ	2.44	0.48
1:A:149:THR:OG1	1:A:528:PRO:HB2	2.14	0.48
1:E:589:PRO:HG2	1:E:674:GLU:HB2	1.96	0.48
1:E:904:ILE:HD11	1:E:942:VAL:HG22	1.94	0.48
1:E:1020:SER:OG	1:E:1023:ASP:OD1	2.30	0.48
1:E:234:ILE:HD13	1:E:277:TYR:O	2.13	0.48
1:A:477:GLY:HA2	1:A:478:LYS:HB3	1.95	0.48
1:A:483:ASP:O	1:A:486:PHE:N	2.45	0.48
1:E:781:TYR:OH	2:F:-19:A:N1	2.36	0.48
1:E:1004:ILE:HG13	1:E:1011:VAL:CG1	2.44	0.47
1:A:105:ILE:HD11	1:A:176:ILE:HD11	1.96	0.47
1:A:461:ASP:OD1	1:A:504:TYR:OH	2.25	0.47
1:A:508:ARG:HB2	1:A:890:TRP:CZ2	2.49	0.47
1:A:640:LYS:HE2	1:A:657:PHE:HB3	1.96	0.47
1:A:756:LEU:HD11	1:A:790:SER:HB3	1.95	0.47
1:A:984:LYS:HE2	3:C:-4:DA:H5''	1.95	0.47
1:E:21:ALA:HB3	1:E:794:TYR:HB3	1.96	0.47
1:E:444:LYS:HE3	1:E:448:LYS:HB3	1.95	0.47
1:A:218:ASP:HB3	1:A:224:PHE:HE1	1.77	0.47
1:A:351:ILE:HG23	1:A:413:LYS:HB3	1.96	0.47
1:A:1:MET:HE3	1:A:2:SER:HA	1.95	0.47
1:E:81:PHE:CZ	1:E:181:THR:HG23	2.48	0.47
1:A:235:ASP:HB3	1:A:287:LEU:HD11	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:LEU:HG	1:A:587:PRO:HD3	1.97	0.47
1:A:1027:PHE:CE1	1:A:1031:PHE:HE1	2.32	0.47
1:A:1058:ASP:O	1:A:1061:LYS:HE2	2.15	0.47
1:E:531:MET:HG3	1:E:544:ALA:HB3	1.97	0.47
1:E:575:ASN:O	1:E:577:ASN:ND2	2.48	0.47
1:E:827:TYR:HE2	1:E:851:VAL:HG21	1.80	0.47
1:E:912:CYS:O	1:E:916:GLU:HG3	2.14	0.47
1:E:1213:ILE:HG12	1:E:1218:TRP:HB2	1.97	0.47
1:A:21:ALA:HB3	1:A:794:TYR:HB3	1.96	0.47
1:E:228:VAL:HG21	1:E:276:LEU:HD12	1.97	0.47
1:E:558:MET:HE3	1:E:566:LEU:HD12	1.96	0.47
1:E:606:TYR:O	1:E:608:PRO:HD3	2.15	0.47
1:E:639:PHE:O	1:E:643:ILE:HG13	2.15	0.47
1:A:706:ASN:ND2	1:A:721:THR:OG1	2.42	0.47
1:A:1004:ILE:HG13	1:A:1011:VAL:CG1	2.45	0.47
1:A:228:VAL:HG21	1:A:276:LEU:HD12	1.97	0.47
1:A:1011:VAL:HG11	1:A:1219:LEU:HD21	1.96	0.47
2:B:-5:U:H2'	2:B:-4:A:H8	1.80	0.47
1:E:595:LYS:NZ	3:G:3:DA:N3	2.60	0.47
1:A:477:GLY:HA3	1:A:479:GLU:HG3	1.96	0.46
1:A:1004:ILE:HG13	1:A:1011:VAL:HG12	1.97	0.46
1:E:161:MET:O	1:E:171:ILE:HG13	2.15	0.46
1:E:314:ILE:O	1:E:318:ILE:HG13	2.15	0.46
1:E:329:ASP:HA	1:E:411:VAL:HG21	1.96	0.46
1:E:965:CYS:O	1:E:972:LYS:NZ	2.48	0.46
1:A:616:TYR:OH	4:D:0:DT:O5'	2.33	0.46
1:E:58:TYR:O	1:E:62:ILE:HG13	2.15	0.46
1:E:1040:GLU:OE1	1:E:1155:LYS:NZ	2.47	0.46
1:A:76:ASN:OD1	1:A:76:ASN:N	2.49	0.46
1:A:924:LEU:O	1:A:996:ILE:HG13	2.16	0.46
2:B:7:A:H2'	2:B:8:G:C8	2.50	0.46
1:E:352:PHE:HE2	1:E:357:VAL:HB	1.80	0.46
1:E:596:VAL:O	1:E:599:SER:OG	2.28	0.46
1:E:1073:ARG:HH22	1:E:1076:ARG:NH2	2.13	0.46
1:E:719:LEU:HB2	1:E:960:LYS:HD3	1.96	0.46
1:E:934:SER:HB3	1:E:938:VAL:CG2	2.46	0.46
1:A:294:TYR:HD2	1:A:300:VAL:HG22	1.80	0.46
1:A:297:ASP:OD2	1:A:446:LEU:HB2	2.16	0.46
1:A:318:ILE:HG23	1:A:466:PHE:CE2	2.50	0.46
1:A:215:ASP:O	1:A:218:ASP:HB2	2.15	0.46
1:A:228:VAL:HG23	1:A:234:ILE:HG12	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:SER:O	1:A:603:MET:N	2.49	0.46
1:E:477:GLY:HA2	1:E:478:LYS:HB3	1.96	0.46
1:A:558:MET:HE3	1:A:566:LEU:HD12	1.97	0.46
1:A:931:PHE:HD1	1:A:931:PHE:O	1.99	0.46
1:A:547:LEU:HD23	1:A:580:LYS:HA	1.97	0.46
1:E:210:LEU:HD23	1:E:210:LEU:HA	1.75	0.46
1:E:215:ASP:HB2	1:E:218:ASP:OD1	2.15	0.46
1:E:663:TYR:CE2	1:E:669:PHE:HB2	2.50	0.46
1:A:294:TYR:CD2	1:A:300:VAL:HG22	2.50	0.46
1:A:1046:ALA:HA	1:A:1064:LYS:HA	1.97	0.46
1:E:988:THR:HG22	1:E:1211:ILE:HD11	1.98	0.46
1:A:161:MET:HE1	1:A:281:LEU:HD22	1.97	0.45
1:A:446:LEU:HD12	1:A:446:LEU:HA	1.84	0.45
1:A:518:LYS:HD2	1:A:748:ARG:HB2	1.97	0.45
1:E:858:GLU:HG2	1:E:871:ASP:HA	1.98	0.45
1:A:21:ALA:O	1:A:794:TYR:HB2	2.16	0.45
1:E:446:LEU:HD12	1:E:446:LEU:HA	1.80	0.45
1:E:909:HIS:CE1	2:F:-3:G:H4'	2.51	0.45
1:E:549:TYR:CE1	1:E:687:LYS:HD2	2.51	0.45
1:A:1192:LEU:HD23	1:A:1195:ILE:HD12	1.97	0.45
1:A:361:LYS:HA	1:A:361:LYS:HD3	1.70	0.45
1:E:325:PHE:O	1:E:328:PHE:HB2	2.16	0.45
1:A:313:GLU:HA	1:A:316:SER:HB3	1.99	0.45
1:A:827:TYR:HE2	1:A:851:VAL:HG21	1.81	0.45
1:E:600:LYS:NZ	3:G:6:DG:OP1	2.49	0.45
1:A:740:GLY:O	3:C:0:DG:H2''	2.17	0.45
1:E:477:GLY:HA3	1:E:479:GLU:HG3	1.98	0.45
1:A:883:ARG:NH2	1:A:894:GLU:O	2.49	0.45
2:B:-1:U:O2'	2:B:1:G:OP1	2.30	0.45
1:E:1090:CYS:HB3	1:E:1093:SER:HB3	1.99	0.45
1:A:397:LEU:HA	1:A:397:LEU:HD23	1.73	0.45
1:E:305:ARG:NH2	1:E:438:ALA:HA	2.30	0.45
1:A:325:PHE:HE1	1:A:473:PHE:HE2	1.64	0.44
1:A:938:VAL:HG12	1:A:940:LYS:N	2.31	0.44
1:A:1005:ASP:OD2	1:A:1152:SER:OG	2.30	0.44
1:E:290:TYR:CE1	3:G:-12:DT:H1'	2.52	0.44
1:E:584:LYS:HA	1:E:584:LYS:HD2	1.72	0.44
1:E:883:ARG:NH2	1:E:894:GLU:O	2.50	0.44
1:E:1127:PHE:HD2	1:E:1128:MET:HE2	1.82	0.44
1:A:457:LYS:HG2	1:A:890:TRP:CE3	2.53	0.44
1:A:620:THR:O	1:A:627:PHE:HA	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:510:TYR:O	1:E:513:GLN:HG2	2.18	0.44
1:E:646:TYR:O	1:E:650:SER:OG	2.22	0.44
2:F:-5:U:H2'	2:F:-4:A:H8	1.81	0.44
1:A:988:THR:HB	1:A:1211:ILE:HD11	1.98	0.44
1:A:1147:VAL:O	1:A:1147:VAL:HG23	2.17	0.44
1:E:228:VAL:HG23	1:E:234:ILE:HA	1.99	0.44
1:A:954:LEU:HD23	1:A:976:ILE:HG13	1.97	0.44
1:E:542:TYR:O	1:E:543:ARG:HB2	2.17	0.44
3:G:5:DG:H2''	3:G:6:DG:O4'	2.16	0.44
1:A:964:PRO:HB3	1:A:970:ALA:HB3	1.98	0.44
1:E:315:PHE:O	1:E:319:LYS:N	2.36	0.44
1:A:187:MET:HG2	1:A:220:PHE:O	2.18	0.44
1:A:842:VAL:HG11	1:A:1185:TYR:HA	1.98	0.44
1:A:189:ILE:O	1:A:193:VAL:HG23	2.17	0.44
1:A:442:LEU:HD23	1:A:442:LEU:HA	1.76	0.44
1:A:726:LEU:HD13	1:A:726:LEU:HA	1.89	0.44
1:A:1040:GLU:OE1	1:A:1155:LYS:NZ	2.46	0.44
2:B:-5:U:H2'	2:B:-4:A:C8	2.52	0.44
1:E:986:MET:CE	1:E:990:ASN:HD22	2.30	0.44
1:E:1031:PHE:CE2	1:E:1047:LEU:HD23	2.52	0.44
1:A:134:ASP:HB3	1:A:137:GLU:HB2	2.00	0.44
1:E:281:LEU:HD12	1:E:281:LEU:HA	1.87	0.44
1:E:349:LYS:HD3	1:E:355:TRP:NE1	2.33	0.44
1:A:302:GLU:HA	1:A:305:ARG:HD3	2.00	0.44
1:A:726:LEU:HD12	1:A:971:LEU:HD11	1.99	0.44
1:A:1049:TYR:O	1:A:1055:THR:OG1	2.32	0.44
1:A:206:LYS:HD2	1:A:214:TYR:O	2.17	0.43
1:A:371:LEU:HD11	1:A:376:VAL:C	2.43	0.43
1:A:534:TRP:O	1:A:583:TYR:HB3	2.18	0.43
1:A:1111:ILE:O	1:A:1115:LEU:HG	2.18	0.43
1:E:838:LEU:HD21	1:E:939:GLU:OE1	2.17	0.43
1:E:998:ALA:O	1:E:1001:THR:OG1	2.31	0.43
1:A:77:TYR:HE1	1:A:98:GLU:HB2	1.82	0.43
1:A:225:PHE:CE2	1:A:229:LEU:HD21	2.52	0.43
1:A:1032:ASP:C	1:A:1112:ARG:NH1	2.76	0.43
1:E:196:ILE:HD11	1:E:259:ILE:HG12	1.99	0.43
1:E:362:TRP:HH2	1:E:388:SER:HB2	1.82	0.43
1:E:663:TYR:OH	1:E:672:GLU:OE2	2.34	0.43
2:F:-12:C:N4	2:F:-11:U:O4	2.51	0.43
1:A:83:LYS:NZ	1:A:85:THR:HG23	2.33	0.43
1:A:505:ASP:OD1	2:B:13:G:O2'	2.36	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1027:PHE:HE1	1:A:1031:PHE:HE1	1.65	0.43
1:E:588:GLY:HA3	1:E:591:LYS:HG3	2.01	0.43
2:F:-5:U:H2'	2:F:-4:A:C8	2.53	0.43
1:A:75:ASN:HD21	1:A:223:GLU:CG	2.28	0.43
1:A:125:GLU:HG2	1:A:145:ASN:OD1	2.17	0.43
1:A:325:PHE:HE1	1:A:473:PHE:CE2	2.36	0.43
1:A:486:PHE:CD2	1:A:487:TYR:HD2	2.29	0.43
1:A:622:LYS:O	1:A:627:PHE:HB2	2.19	0.43
1:E:72:LYS:HG3	1:E:104:GLU:OE2	2.18	0.43
1:E:471:LYS:HB3	1:E:471:LYS:HE2	1.90	0.43
1:E:1073:ARG:NH2	1:E:1087:GLU:OE1	2.51	0.43
1:A:752:LYS:CB	1:A:755:GLU:HG3	2.46	0.43
1:A:843:VAL:HG11	1:A:918:TYR:CD2	2.54	0.43
1:A:876:LEU:HD23	1:A:899:LEU:HG	2.00	0.43
1:E:80:LEU:HD23	1:E:94:LEU:HB2	2.01	0.43
1:E:640:LYS:HE2	1:E:657:PHE:HB3	2.00	0.43
1:E:657:PHE:CZ	1:E:673:VAL:HG22	2.54	0.43
1:A:84:LYS:HE2	1:A:84:LYS:H	1.84	0.43
1:A:817:ARG:HB3	1:A:1206:LEU:CD2	2.49	0.43
1:E:838:LEU:HA	1:E:838:LEU:HD23	1.82	0.43
1:E:931:PHE:HD1	1:E:931:PHE:O	2.01	0.43
1:A:144:PHE:HD2	1:A:151:PHE:HE1	1.66	0.43
1:A:234:ILE:HD13	1:A:277:TYR:O	2.19	0.43
1:A:244:PHE:CE2	1:A:246:THR:HG22	2.53	0.43
1:A:591:LYS:HB2	4:D:-1:DA:HI'	2.00	0.43
1:A:986:MET:CE	1:A:990:ASN:HD22	2.27	0.43
1:A:1192:LEU:HD23	1:A:1192:LEU:HA	1.84	0.43
1:E:121:LYS:HD2	1:E:125:GLU:OE2	2.19	0.43
1:E:138:ILE:HD12	1:E:138:ILE:HA	1.89	0.43
1:A:900:LYS:O	1:A:904:ILE:HG12	2.18	0.43
1:E:308:LEU:HD12	1:E:459:LEU:CD2	2.49	0.43
1:E:1011:VAL:HG23	1:E:1013:LEU:HG	2.00	0.43
1:E:1052:PHE:HB2	1:E:1055:THR:HG21	2.01	0.43
1:A:239:ALA:O	1:A:243:GLY:N	2.46	0.42
1:A:904:ILE:HD12	1:A:946:PHE:HA	2.01	0.42
2:B:7:A:H2'	2:B:8:G:H8	1.82	0.42
1:A:80:LEU:HG	1:A:94:LEU:HD12	2.01	0.42
1:A:228:VAL:HG21	1:A:276:LEU:CD1	2.48	0.42
1:A:314:ILE:HD13	1:A:500:VAL:HG12	2.00	0.42
1:A:349:LYS:HD3	1:A:355:TRP:NE1	2.33	0.42
1:A:1011:VAL:HG23	1:A:1013:LEU:HG	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:167:LYS:NZ	3:G:-2:DG:OP1	2.29	0.42
1:E:1000:LEU:HD23	1:E:1000:LEU:HA	1.86	0.42
1:E:1160:ILE:HD12	1:E:1161:PHE:H	1.84	0.42
2:F:11:A:H2'	2:F:12:A:C8	2.53	0.42
1:A:328:PHE:HB3	1:A:411:VAL:HG23	2.01	0.42
1:A:633:HIS:CE1	1:A:661:GLU:HA	2.54	0.42
1:E:387:LYS:HD3	1:E:388:SER:N	2.34	0.42
1:A:179:ASN:HD21	1:A:234:ILE:HD11	1.85	0.42
1:A:352:PHE:HB3	1:A:408:LEU:CD1	2.49	0.42
1:A:352:PHE:HB3	1:A:408:LEU:HD13	2.00	0.42
1:A:379:GLU:O	1:A:383:ASP:HB2	2.20	0.42
1:A:505:ASP:OD1	1:A:508:ARG:NH2	2.53	0.42
1:E:139:ALA:HA	1:E:142:ASN:ND2	2.35	0.42
1:E:163:SER:HB3	1:E:170:SER:HB2	2.01	0.42
1:E:263:ASN:ND2	1:E:270:LEU:H	2.18	0.42
1:E:361:LYS:HD3	1:E:361:LYS:HA	1.79	0.42
1:E:876:LEU:CD2	1:E:899:LEU:HG	2.48	0.42
2:F:7:A:H2'	2:F:8:G:C8	2.54	0.42
1:A:281:LEU:HD12	1:A:281:LEU:HA	1.91	0.42
1:A:290:TYR:CE1	3:C:-12:DT:H1'	2.53	0.42
1:A:486:PHE:CD2	1:A:487:TYR:CD2	3.06	0.42
1:A:555:LEU:N	1:A:702:PHE:O	2.40	0.42
1:E:938:VAL:HG12	1:E:940:LYS:N	2.34	0.42
1:A:200:HIS:O	1:A:204:GLU:N	2.38	0.42
1:A:376:VAL:O	1:A:377:VAL:HG13	2.19	0.42
1:A:589:PRO:HG2	1:A:674:GLU:HB2	2.02	0.42
1:E:527:ASN:HB2	1:E:543:ARG:NH1	2.35	0.42
1:A:58:TYR:O	1:A:62:ILE:HG13	2.19	0.42
1:A:1047:LEU:HB2	1:A:1052:PHE:HE1	1.84	0.42
1:E:534:TRP:O	1:E:583:TYR:HB3	2.19	0.42
1:E:954:LEU:HD23	1:E:976:ILE:HG13	2.00	0.42
3:G:-11:DT:H2'	3:G:-10:DT:C6	2.54	0.42
1:A:81:PHE:CZ	1:A:181:THR:HG23	2.53	0.42
1:A:387:LYS:HE3	1:A:391:LYS:HE2	2.00	0.42
1:A:414:LEU:HD11	1:A:473:PHE:HZ	1.85	0.42
1:E:51:LYS:HG2	1:E:154:PHE:CE2	2.55	0.42
1:E:95:GLU:O	1:E:99:ILE:HG13	2.20	0.42
1:A:413:LYS:O	1:A:417:ILE:HG13	2.20	0.42
1:E:442:LEU:HD23	1:E:442:LEU:HA	1.84	0.42
1:E:505:ASP:OD1	2:F:13:G:O2'	2.29	0.42
1:E:904:ILE:HD12	1:E:946:PHE:HA	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:TYR:CE1	1:A:687:LYS:HD2	2.55	0.42
1:A:610:GLU:HG2	1:A:611:ASP:N	2.35	0.42
1:A:636:ILE:O	1:A:640:LYS:HG3	2.20	0.42
1:A:1160:ILE:HD12	1:A:1161:PHE:H	1.85	0.42
1:A:936:VAL:O	1:A:938:VAL:HG22	2.19	0.41
1:E:128:LEU:HD23	1:E:141:VAL:HG21	2.02	0.41
1:E:325:PHE:CD1	1:E:418:ILE:HG12	2.54	0.41
1:A:535:ASP:OD2	3:C:2:DA:H5''	2.20	0.41
2:B:-3:G:H2'	2:B:-2:A:O4'	2.20	0.41
1:E:1213:ILE:HG13	1:E:1214:SER:O	2.20	0.41
1:E:208:LYS:HG3	1:E:252:ILE:HD12	2.03	0.41
1:E:415:LYS:HG2	1:E:419:ILE:HD12	2.02	0.41
1:E:447:LYS:HG3	1:E:513:GLN:O	2.21	0.41
1:E:1071:ARG:O	1:E:1088:GLU:HA	2.19	0.41
1:A:310:LYS:HA	1:A:315:PHE:CD2	2.55	0.41
1:A:322:GLU:OE2	1:A:419:ILE:HG22	2.20	0.41
1:A:858:GLU:OE2	1:A:869:LYS:HD3	2.20	0.41
1:E:168:SER:HA	1:E:173:PHE:CD2	2.56	0.41
1:E:1219:LEU:HD23	1:E:1219:LEU:HA	1.84	0.41
1:A:180:LEU:HD23	1:A:180:LEU:HA	1.88	0.41
1:A:425:ILE:HD11	1:A:466:PHE:CB	2.50	0.41
1:A:542:TYR:O	1:A:543:ARG:HB2	2.19	0.41
1:A:648:LYS:HB2	1:A:648:LYS:HE3	1.91	0.41
1:E:84:LYS:HA	1:E:84:LYS:HD3	1.87	0.41
1:E:206:LYS:HD3	1:E:215:ASP:HA	2.01	0.41
1:E:673:VAL:O	1:E:677:GLY:N	2.53	0.41
1:A:309:ASN:ND2	1:A:309:ASN:H	2.18	0.41
1:E:155:PHE:O	1:E:159:GLU:HG3	2.20	0.41
1:E:1062:LYS:HE3	1:E:1062:LYS:HB2	1.85	0.41
1:E:1131:MET:O	1:E:1135:LEU:HD12	2.20	0.41
1:A:72:LYS:HG3	1:A:104:GLU:CD	2.46	0.41
1:A:46:ASP:O	1:A:50:VAL:HG23	2.20	0.41
1:A:124:ILE:HG23	1:A:141:VAL:HG13	2.02	0.41
1:A:640:LYS:NZ	1:A:660:THR:OG1	2.31	0.41
1:A:1021:ILE:HG23	1:A:1124:TYR:CE2	2.56	0.41
1:A:1073:ARG:HH12	1:A:1076:ARG:HH21	1.68	0.41
1:A:1137:MET:O	1:A:1150:LEU:HD12	2.20	0.41
1:E:331:TYR:CD2	1:E:486:PHE:HD1	2.39	0.41
1:E:1196:GLY:O	1:E:1200:LYS:HG3	2.21	0.41
1:A:71:LEU:HD13	1:A:71:LEU:HA	1.89	0.41
1:A:198:ASP:OD1	1:A:199:LYS:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:LYS:HE2	1:A:511:VAL:O	2.21	0.41
1:A:475:GLY:C	1:A:476:GLU:HG3	2.46	0.41
1:A:584:LYS:HA	1:A:584:LYS:HD2	1.69	0.41
1:A:1010:PHE:HB2	1:A:1063:TRP:CZ3	2.56	0.41
3:C:5:DG:H2''	3:C:6:DG:O4'	2.20	0.41
1:E:379:GLU:O	1:E:383:ASP:HB2	2.21	0.41
1:E:469:TYR:HD2	1:E:470:ILE:HD12	1.85	0.41
1:E:477:GLY:HA3	1:E:479:GLU:OE2	2.21	0.41
1:A:844:VAL:HA	1:A:849:ASN:O	2.20	0.41
1:E:616:TYR:OH	4:H:0:DT:O5'	2.38	0.41
1:E:844:VAL:HA	1:E:849:ASN:O	2.21	0.41
1:A:192:LYS:NZ	1:A:270:LEU:HD22	2.36	0.40
1:A:1091:LEU:HD13	1:A:1134:MET:HG2	2.03	0.40
1:E:208:LYS:HD3	1:E:208:LYS:HA	1.88	0.40
1:E:613:GLN:H	1:E:613:GLN:HG3	1.67	0.40
1:A:471:LYS:HB3	1:A:471:LYS:HE2	1.94	0.40
1:A:1023:ASP:OD1	1:A:1023:ASP:N	2.55	0.40
1:A:1076:ARG:H	1:A:1076:ARG:HE	1.69	0.40
1:E:502:HIS:O	1:E:502:HIS:ND1	2.53	0.40
1:A:418:ILE:O	1:A:422:VAL:HG13	2.21	0.40
1:A:435:LEU:HD23	1:A:455:ILE:HG21	2.03	0.40
1:A:756:LEU:O	1:A:758:VAL:HG23	2.21	0.40
1:A:1111:ILE:HG22	1:A:1115:LEU:HG	2.04	0.40
1:A:1174:ILE:HD12	1:A:1174:ILE:HA	1.92	0.40
1:E:337:PHE:CG	1:E:479:GLU:OE1	2.75	0.40
1:E:565:CYS:SG	1:E:566:LEU:N	2.94	0.40
1:E:843:VAL:HG11	1:E:918:TYR:CD2	2.57	0.40
1:A:100:ASN:HA	1:A:103:LYS:HB2	2.03	0.40
1:A:155:PHE:O	1:A:159:GLU:HG3	2.22	0.40
1:A:572:ASP:O	1:A:577:ASN:ND2	2.52	0.40
1:A:767:ASN:ND2	1:A:774:LYS:O	2.38	0.40
1:A:939:GLU:O	1:A:942:VAL:HG12	2.22	0.40
1:A:1072:ILE:HD13	1:A:1141:ILE:HD11	2.02	0.40
1:E:294:TYR:HD2	1:E:300:VAL:HG22	1.86	0.40
1:E:726:LEU:HB3	1:E:971:LEU:HD21	2.04	0.40
1:E:1110:ASP:C	1:E:1111:ILE:HD13	2.46	0.40
1:A:120:LYS:O	1:A:123:ILE:HG22	2.22	0.40
1:A:413:LYS:NZ	1:A:416:GLU:OE1	2.33	0.40
1:A:1112:ARG:HH11	1:A:1112:ARG:HD3	1.73	0.40
1:E:52:LYS:HD2	1:E:52:LYS:HA	1.69	0.40
1:E:134:ASP:HB3	1:E:137:GLU:HB2	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:354:GLU:HB3	1:E:357:VAL:HG23	2.04	0.40
1:E:455:ILE:HD13	1:E:455:ILE:HA	1.92	0.40
1:E:696:GLU:OE1	1:E:698:LYS:HE3	2.21	0.40
1:E:964:PRO:HA	1:E:969:GLY:HA3	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:332:SER:OG	1:E:637:ASP:OD2[2_545]	2.14	0.06

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	1219/1228 (99%)	1187 (97%)	31 (2%)	1 (0%)	48 78
1	E	1219/1228 (99%)	1186 (97%)	32 (3%)	1 (0%)	48 78
All	All	2438/2456 (99%)	2373 (97%)	63 (3%)	2 (0%)	48 78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	377	VAL
1	A	377	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	1076/1115 (96%)	1075 (100%)	1 (0%)	88	87
1	E	1076/1115 (96%)	1076 (100%)	0	100	100
All	All	2152/2230 (96%)	2151 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	370	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	231	GLN
1	A	401	GLN
1	A	420	GLN
1	A	449	ASN
1	A	628	ASN
1	A	955	ASN
1	A	1197	GLN
1	E	73	ASN
1	E	75	ASN
1	E	142	ASN
1	E	231	GLN
1	E	513	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	34/40 (85%)	4 (11%)	0
2	F	34/40 (85%)	4 (11%)	0
All	All	68/80 (85%)	8 (11%)	0

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	-12	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	-10	A
2	B	-9	A
2	B	-6	G
2	F	-12	C
2	F	-10	A
2	F	-9	A
2	F	-6	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1223/1228 (99%)	0.40	26 (2%) 63 38	7, 47, 90, 133	0
1	E	1223/1228 (99%)	0.38	27 (2%) 62 37	8, 47, 104, 136	0
2	B	35/40 (87%)	0.52	0 100 100	11, 19, 44, 60	0
2	F	35/40 (87%)	0.54	0 100 100	10, 21, 50, 64	0
3	C	23/23 (100%)	0.89	2 (8%) 16 12	24, 44, 98, 133	0
3	G	23/23 (100%)	0.84	3 (13%) 7 7	26, 43, 101, 144	0
4	D	11/11 (100%)	0.89	0 100 100	42, 47, 102, 108	0
4	H	11/11 (100%)	1.18	1 (9%) 15 11	49, 56, 117, 124	0
All	All	2584/2604 (99%)	0.41	59 (2%) 61 37	7, 47, 100, 144	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	376	VAL	4.5
1	A	376	VAL	4.5
1	E	347	ILE	3.9
1	E	939	GLU	3.8
1	E	381	TYR	3.7
1	E	835	GLU	3.4
1	E	291	GLY	3.3
4	H	-9	DC	3.3
1	A	377	VAL	3.2
1	A	938	VAL	2.9
1	E	469	TYR	2.9
1	A	632	CYS	2.9
1	A	714	HIS	2.8
1	E	293	GLY	2.8
1	A	291	GLY	2.8
1	A	527	ASN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	452	VAL	2.7
1	E	938	VAL	2.7
1	E	473	PHE	2.7
1	E	111	GLY	2.7
3	C	-13	DC	2.7
1	A	469	TYR	2.6
1	E	466	PHE	2.6
1	A	1056	ASP	2.6
1	A	195	ALA	2.6
3	C	7	DA	2.6
1	A	333	SER	2.6
3	G	-13	DC	2.5
1	A	1218	TRP	2.5
1	A	1077	ASN	2.5
1	E	195	ALA	2.5
1	E	983	PHE	2.5
1	E	202	VAL	2.5
1	E	377	VAL	2.5
1	E	271	PRO	2.4
1	E	243	GLY	2.4
1	E	77	TYR	2.4
1	A	381	TYR	2.4
1	A	834	GLY	2.3
3	G	9	DG	2.3
1	A	835	GLU	2.3
1	E	528	PRO	2.3
1	E	432	SER	2.3
1	E	149	THR	2.3
1	A	328	PHE	2.2
1	A	833	ARG	2.2
1	A	1069	GLY	2.2
1	E	516	TYR	2.2
1	A	902	GLY	2.1
1	E	430	GLY	2.1
1	A	566	LEU	2.1
1	E	401	GLN	2.1
1	A	429	TYR	2.1
3	G	7	DA	2.1
1	E	248	SER	2.1
1	A	271	PRO	2.0
1	A	516	TYR	2.0
1	A	556	ALA	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1082	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	LI	A	1302	1/1	0.38	0.87	10,10,10,10	0
5	LI	A	1301	1/1	0.76	1.53	9,9,9,9	0
5	LI	B	101	1/1	0.87	1.01	5,5,5,5	0

6.5 Other polymers [i](#)

There are no such residues in this entry.