



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2023 – 07:23 PM EDT

PDB ID : 2DU6
Title : Crystal structure of Archaeoglobus fulgidus O-phosphoseryl-tRNA synthetase E418N/E420N mutant complexed with tRNA^{Amber} and O-phosphoserine ("amber complex")
Authors : Fukunaga, R.
Deposited on : 2006-07-20
Resolution : 3.30 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

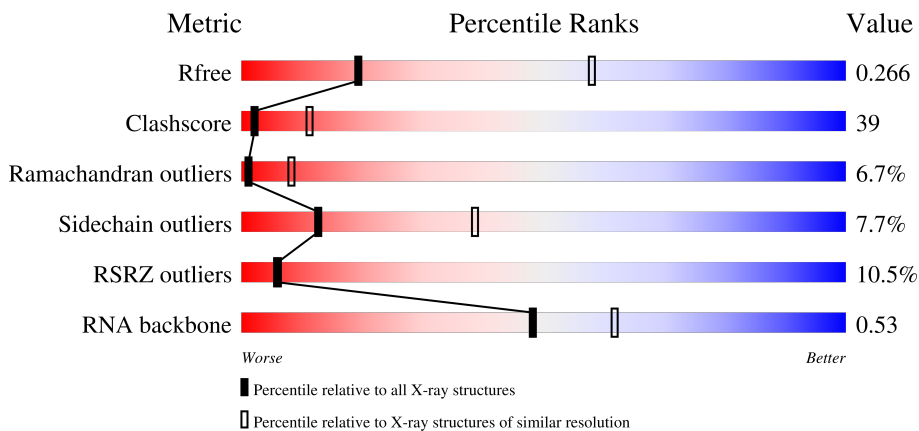
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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	D	71	Upper bar: 82% Lower bar: 41% (red), 38% (orange), 20% (yellow), 1% (green), 0% (grey)
2	A	534	Upper bar: 8% Lower bar: 35% (red), 54% (orange), 10% (yellow), 1% (green), 0% (grey)
2	B	534	Upper bar: 2% Lower bar: 32% (red), 47% (orange), 7% (yellow), 13% (grey)

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9619 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 RNA chain called tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	D	71	1517	674	269	503	71	0	0	0

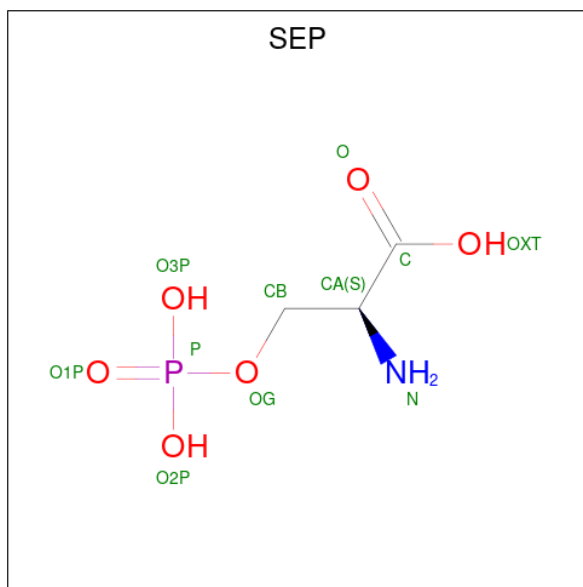
- Molecule 2 is a protein called O-phosphoseryl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	534	4319	2784	721	801	13	0	0	0
2	B	465	3761	2427	632	689	13	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	418	ASN	GLU	engineered mutation	UNP O30126
A	420	ASN	GLU	engineered mutation	UNP O30126
B	418	ASN	GLU	engineered mutation	UNP O30126
B	420	ASN	GLU	engineered mutation	UNP O30126

- Molecule 3 is PHOSPHOSERINE (three-letter code: SEP) (formula: C₃H₈NO₆P).

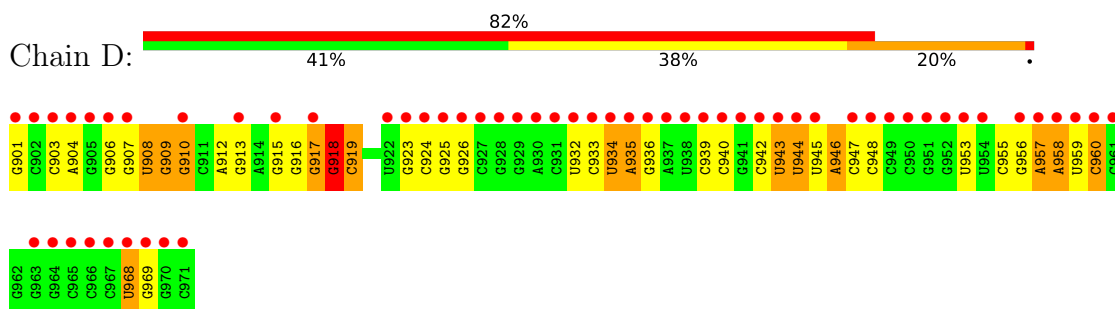


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	11	3	1	6	1	0	0
3	A	1	11	3	1	6	1	0	0

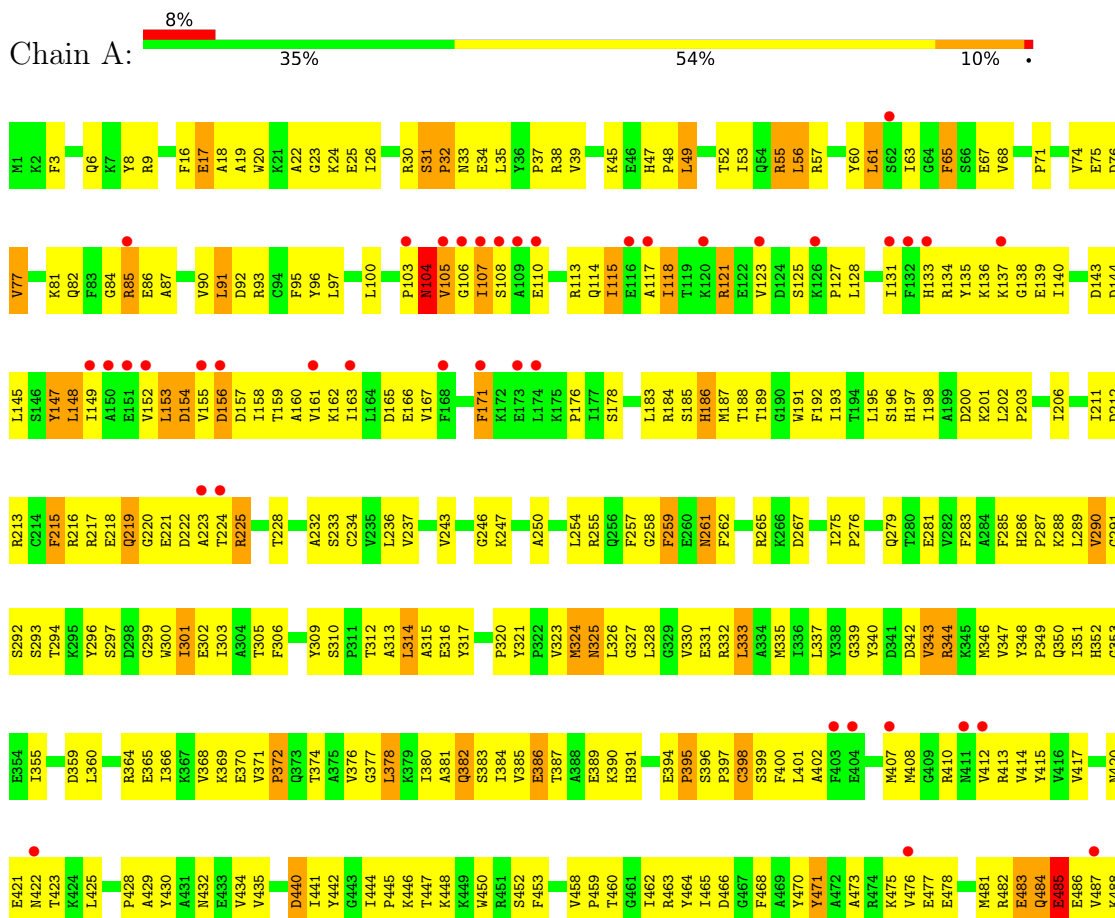
3 Residue-property plots

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: tRNA

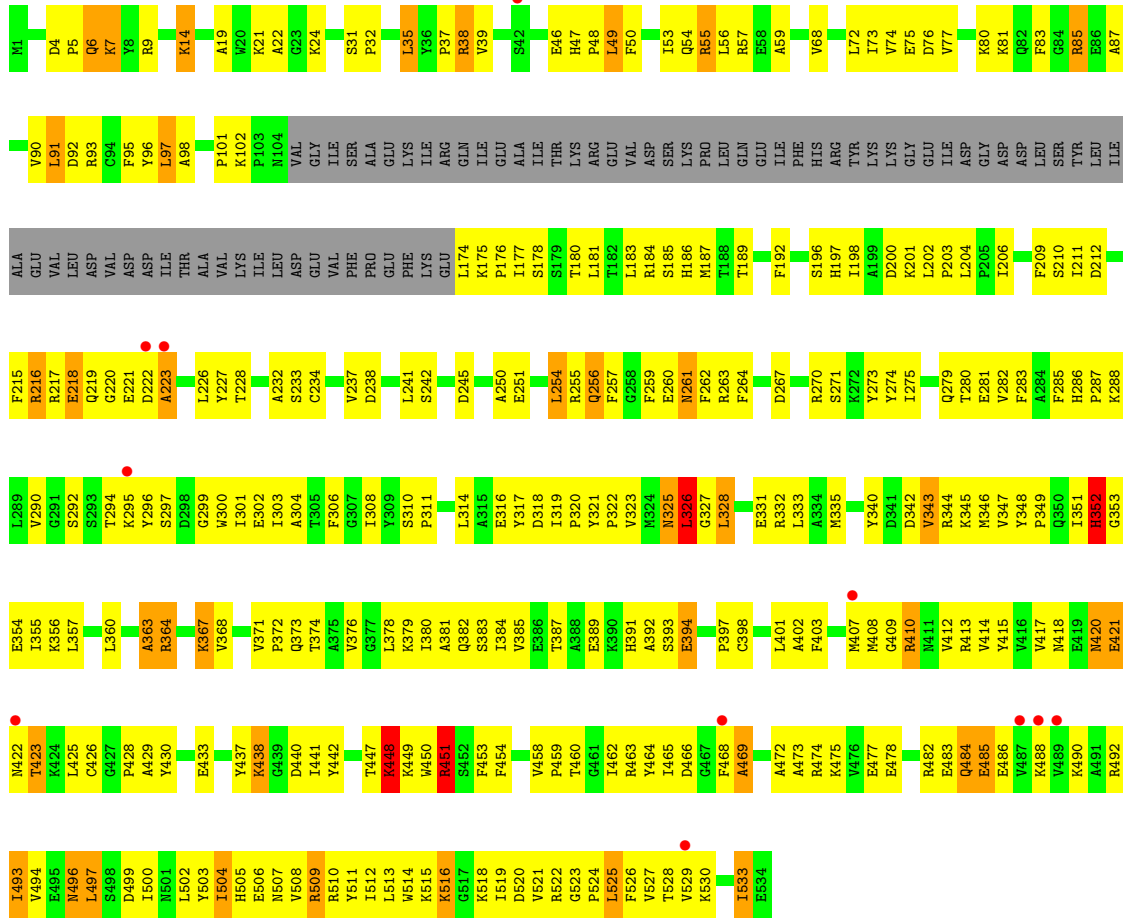


• Molecule 2: O-phosphoseryl-tRNA synthetase





● Molecule 2: O-phosphoseryl-tRNA synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	148.32Å 148.32Å 152.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.14 – 3.30 49.14 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.14-3.30) 99.8 (49.14-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 3.33Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.265 , 0.329 0.202 , 0.266	Depositor DCC
R_{free} test set	1458 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	95.8	Xtrriage
Anisotropy	0.076	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 119.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	0.053 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9619	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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: SEP

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	D	0.31	1/1693 (0.1%)	0.68	0/2637
2	A	0.32	0/4416	0.56	0/5966
2	B	0.33	0/3849	0.61	1/5200 (0.0%)
All	All	0.32	1/9958 (0.0%)	0.60	1/13803 (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	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	901	G	OP3-P	-7.12	1.52	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	326	LEU	CA-CB-CG	5.18	127.22	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	918	G	Sidechain

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	D	1517	0	768	41	0
2	A	4319	0	4339	401	0
2	B	3761	0	3774	318	0
3	A	22	0	10	3	0
All	All	9619	0	8891	731	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 39.

All (731) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:ARG:HG2	2:B:218:GLU:HG2	1.37	1.06
2:A:148:LEU:HG	2:A:160:ALA:HB2	1.34	1.06
2:B:448:LYS:H	2:B:448:LYS:HD3	1.15	1.05
1:D:957:A:H1'	1:D:959:U:H5	1.23	1.03
2:B:232:ALA:HB3	2:B:328:LEU:HB3	1.41	1.02
2:B:267:ASP:HB3	2:B:279:GLN:HG2	1.42	1.00
2:B:47:HIS:HD2	2:B:49:LEU:H	1.15	0.94
2:A:381:ALA:HB2	2:A:473:ALA:HB2	1.48	0.94
2:A:533:ILE:HD13	2:A:533:ILE:H	1.32	0.94
2:B:254:LEU:HD21	2:B:303:ILE:HG21	1.48	0.94
2:A:224:THR:O	2:A:225:ARG:HB2	1.69	0.92
2:B:263:ARG:HG2	2:B:300:TRP:CZ3	2.06	0.91
2:B:346:MET:O	2:B:349:PRO:HD3	1.71	0.90
2:B:254:LEU:HD21	2:B:303:ILE:CG2	2.02	0.89
2:A:397:PRO:HD3	2:A:421:GLU:HG2	1.54	0.89
2:A:223:ALA:HA	2:A:344:ARG:HD2	1.53	0.89
2:A:301:ILE:HD11	2:A:332:ARG:HD3	1.53	0.88
2:A:328:LEU:HD11	2:A:333:LEU:HD12	1.55	0.86
2:A:33:ASN:HA	2:A:38:ARG:HD2	1.57	0.86
1:D:942:C:O2'	1:D:943:U:H5'	1.76	0.84
2:A:460:THR:HG23	2:A:462:ILE:H	1.41	0.84
2:B:464:TYR:HA	2:B:500:ILE:HD11	1.60	0.83
2:B:381:ALA:HB1	2:B:469:ALA:HB1	1.59	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:957:A:HI'	1:D:959:U:C5	2.12	0.83
2:B:385:VAL:HG13	2:B:465:ILE:HD12	1.62	0.82
2:A:128:LEU:HD23	2:A:128:LEU:H	1.46	0.81
2:A:380:ILE:O	2:A:384:ILE:HG13	1.81	0.81
2:A:434:VAL:HB	2:A:460:THR:HG21	1.63	0.80
2:B:355:ILE:O	2:B:515:LYS:HE3	1.81	0.80
2:A:510:ARG:HH21	2:B:200:ASP:HB2	1.46	0.80
2:B:412:VAL:HG22	2:B:533:ILE:HG22	1.64	0.79
2:B:206:ILE:HB	2:B:237:VAL:HB	1.64	0.79
2:A:206:ILE:HB	2:A:237:VAL:HB	1.62	0.79
2:B:533:ILE:H	2:B:533:ILE:HD13	1.48	0.78
2:B:448:LYS:HD3	2:B:448:LYS:N	1.97	0.78
2:A:351:ILE:HG22	2:A:352:HIS:HD2	1.46	0.78
2:B:294:THR:HG23	2:B:296:TYR:H	1.50	0.76
2:B:196:SER:HA	2:B:319:ILE:HD11	1.67	0.76
2:A:158:ILE:HG13	2:A:159:THR:HG23	1.67	0.76
2:A:267:ASP:HB3	2:A:279:GLN:HG2	1.66	0.75
2:B:368:VAL:HA	2:B:502:LEU:HD12	1.68	0.75
2:A:6:GLN:HA	2:A:9:ARG:HH11	1.51	0.75
2:A:294:THR:HG23	2:A:296:TYR:H	1.49	0.75
2:A:410:ARG:CZ	2:A:483:GLU:HG3	2.17	0.75
2:A:186:HIS:NE2	2:A:188:THR:HB	2.02	0.75
2:B:407:MET:HE1	2:B:477:GLU:HA	1.68	0.74
2:A:407:MET:HB3	2:A:412:VAL:HG21	1.69	0.74
2:A:222:ASP:OD2	2:A:344:ARG:HG2	1.88	0.73
2:A:178:SER:HB3	2:B:176:PRO:HB2	1.69	0.73
2:B:372:PRO:HB2	2:B:378:LEU:HD22	1.71	0.73
2:B:219:GLN:HB3	2:B:221:GLU:HG3	1.70	0.72
2:A:75:GLU:HB3	2:A:77:VAL:HG13	1.71	0.72
2:A:193:ILE:O	2:A:196:SER:HB3	1.89	0.72
2:B:53:ILE:HG23	2:B:211:ILE:HG21	1.71	0.72
2:A:447:THR:HG22	2:A:448:LYS:H	1.55	0.72
2:A:490:LYS:HB3	2:A:528:THR:HG23	1.72	0.71
2:B:47:HIS:CD2	2:B:49:LEU:H	2.05	0.71
2:B:448:LYS:H	2:B:448:LYS:CD	1.91	0.71
2:A:91:LEU:H	2:A:91:LEU:HD12	1.55	0.71
2:A:110:GLU:HG2	2:A:114:GLN:HE21	1.54	0.71
2:A:303:ILE:HD11	2:A:333:LEU:HG	1.72	0.71
2:B:504:ILE:HB	2:B:508:VAL:HG21	1.71	0.71
2:A:333:LEU:O	2:A:337:LEU:HG	1.89	0.71
2:B:222:ASP:O	2:B:344:ARG:HD3	1.90	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:287:PRO:O	2:A:290:VAL:HG22	1.91	0.71
2:B:376:VAL:HA	2:B:379:LYS:HE2	1.70	0.71
2:A:301:ILE:HD13	2:A:302:GLU:N	2.06	0.71
2:A:144:ASP:HA	2:A:147:TYR:CZ	2.25	0.70
2:B:72:LEU:HA	2:B:184:ARG:NH2	2.07	0.70
2:A:504:ILE:HB	2:A:508:VAL:HG21	1.74	0.70
2:B:441:ILE:HB	2:B:519:ILE:HG23	1.72	0.70
2:A:478:GLU:HB3	2:A:482:ARG:HH22	1.57	0.69
2:B:6:GLN:HG2	2:B:9:ARG:HH11	1.57	0.69
2:A:37:PRO:O	2:A:364:ARG:HG3	1.93	0.69
2:A:97:LEU:HD11	2:A:183:LEU:HG	1.75	0.69
2:A:507:ASN:HD21	2:B:200:ASP:HA	1.58	0.68
2:B:381:ALA:HA	2:B:384:ILE:HG12	1.76	0.68
2:A:325:ASN:HD22	2:A:326:LEU:N	1.91	0.68
2:A:376:VAL:HG12	2:A:380:ILE:CD1	2.24	0.68
2:A:275:ILE:HG23	2:A:276:PRO:HD2	1.75	0.68
1:D:915:G:H2'	1:D:916:G:O4'	1.93	0.68
2:A:494:VAL:O	2:A:522:ARG:HA	1.94	0.68
1:D:959:U:H5'	1:D:960:C:OP2	1.94	0.68
2:A:97:LEU:HD23	2:B:95:PHE:CE2	2.29	0.68
2:A:511:TYR:HB2	2:B:201:LYS:O	1.94	0.68
2:B:237:VAL:HG22	2:B:323:VAL:HG22	1.76	0.68
2:B:215:PHE:CD2	2:B:228:THR:HG22	2.28	0.67
2:B:280:THR:HG22	2:B:281:GLU:H	1.59	0.67
2:B:202:LEU:HB2	2:B:206:ILE:HD11	1.77	0.67
1:D:917:G:H4'	1:D:918:G:OP1	1.93	0.67
1:D:934:U:H4'	1:D:935:A:OP2	1.93	0.67
2:B:392:ALA:HB1	2:B:426:CYS:HB2	1.75	0.67
2:A:3:PHE:HD2	2:A:26:ILE:HG21	1.60	0.67
2:A:57:ARG:O	2:A:61:LEU:HD12	1.95	0.67
2:B:290:VAL:HA	2:B:297:SER:O	1.94	0.67
2:B:19:ALA:O	2:B:22:ALA:HB3	1.95	0.66
1:D:925:G:H2'	1:D:926:G:C8	2.29	0.66
2:A:213:ARG:HH21	2:A:228:THR:CG2	2.07	0.66
2:A:258:GLY:HA3	2:A:286:HIS:CE1	2.30	0.66
2:A:434:VAL:HB	2:A:460:THR:CG2	2.25	0.66
1:D:953:U:H3	1:D:957:A:H62	1.44	0.66
2:B:343:VAL:O	2:B:347:VAL:HG12	1.95	0.66
2:A:76:ASP:HB2	2:A:91:LEU:HD21	1.77	0.66
2:B:175:LYS:HD2	2:B:175:LYS:N	2.11	0.66
2:B:497:LEU:HD13	2:B:509:ARG:HH12	1.61	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:325:ASN:HD22	2:A:325:ASN:C	1.98	0.65
2:A:508:VAL:HG12	2:B:203:PRO:HG3	1.77	0.65
2:B:242:SER:O	2:B:308:ILE:HD11	1.97	0.65
2:A:410:ARG:NH2	2:A:483:GLU:HG3	2.10	0.65
2:A:33:ASN:HA	2:A:38:ARG:CD	2.25	0.65
2:A:447:THR:HG22	2:A:448:LYS:N	2.12	0.65
2:B:254:LEU:O	2:B:259:PHE:HD1	1.79	0.65
2:A:77:VAL:O	2:A:81:LYS:HG3	1.97	0.64
2:B:433:GLU:OE2	2:B:459:PRO:HB2	1.98	0.64
2:A:496:ASN:ND2	2:A:499:ASP:H	1.95	0.64
2:A:432:ASN:O	2:A:463:ARG:HA	1.97	0.64
2:A:188:THR:HG23	2:A:309:TYR:OH	1.98	0.64
1:D:968:U:H2'	1:D:969:G:C8	2.33	0.64
2:A:376:VAL:HG12	2:A:380:ILE:HD11	1.79	0.64
2:A:505:HIS:O	2:A:508:VAL:HG22	1.96	0.64
2:B:250:ALA:O	2:B:254:LEU:HB2	1.97	0.64
2:B:363:ALA:HB2	2:B:458:VAL:CG2	2.28	0.63
2:B:381:ALA:HB2	2:B:473:ALA:HB2	1.80	0.63
2:A:236:LEU:HB3	2:A:324:MET:HB3	1.79	0.63
2:A:325:ASN:C	2:A:325:ASN:ND2	2.50	0.63
2:A:200:ASP:HA	2:B:507:ASN:ND2	2.13	0.63
3:A:1002:SEP:HB2	2:B:327:GLY:HA3	1.80	0.63
2:B:497:LEU:HD12	2:B:497:LEU:H	1.63	0.63
2:A:283:PHE:CE1	2:A:302:GLU:HB2	2.33	0.63
2:B:376:VAL:HA	2:B:379:LYS:CE	2.29	0.63
2:B:35:LEU:HD12	2:B:35:LEU:H	1.63	0.63
2:B:174:LEU:HB3	2:B:175:LYS:HD2	1.80	0.63
2:B:335:MET:SD	2:B:343:VAL:HG23	2.38	0.63
2:A:91:LEU:HD23	2:A:96:TYR:OH	1.99	0.63
2:A:200:ASP:HB2	2:B:510:ARG:HE	1.64	0.63
2:A:296:TYR:CE2	2:A:301:ILE:HG12	2.33	0.62
2:A:492:ARG:HH11	2:A:492:ARG:HG3	1.63	0.62
2:B:81:LYS:HD3	2:B:316:GLU:HG3	1.80	0.62
1:D:943:U:H2'	1:D:944:U:H5'	1.79	0.62
2:B:384:ILE:HD12	2:B:414:VAL:HG11	1.81	0.62
2:B:458:VAL:HG23	2:B:458:VAL:O	1.98	0.62
2:B:488:LYS:HG3	2:B:530:LYS:HG2	1.82	0.62
2:A:485:GLU:HA	2:A:533:ILE:O	1.99	0.62
2:A:6:GLN:HA	2:A:9:ARG:NH1	2.14	0.62
2:B:475:LYS:HD2	2:B:478:GLU:OE2	1.99	0.62
2:B:437:TYR:CE2	2:B:438:LYS:HG2	2.35	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:ARG:O	2:B:217:ARG:HB3	2.00	0.62
2:A:139:GLU:HB3	2:A:143:ASP:OD1	2.00	0.61
2:A:328:LEU:CD1	2:A:333:LEU:HD12	2.26	0.61
2:B:508:VAL:O	2:B:511:TYR:HB3	1.98	0.61
2:B:251:GLU:HG3	2:B:262:PHE:CE2	2.35	0.61
2:B:282:VAL:HG22	2:B:304:ALA:O	2.00	0.61
2:A:38:ARG:NH2	2:A:462:ILE:HD11	2.15	0.61
2:A:160:ALA:HA	2:A:163:ILE:HG22	1.82	0.61
2:A:401:LEU:HD13	2:A:415:TYR:HE1	1.66	0.61
2:A:434:VAL:HG21	2:A:502:LEU:CD2	2.29	0.61
2:A:121:ARG:O	2:A:123:VAL:HG13	2.01	0.61
2:A:219:GLN:O	2:A:221:GLU:N	2.33	0.61
2:A:309:TYR:HB2	2:A:323:VAL:HG13	1.83	0.61
2:A:306:PHE:HB3	2:A:326:LEU:HD22	1.82	0.61
2:A:135:TYR:HA	2:A:139:GLU:CG	2.31	0.60
2:A:285:PHE:HB2	2:A:300:TRP:CE2	2.36	0.60
2:B:217:ARG:O	2:B:217:ARG:HG2	2.01	0.60
2:A:445:PRO:O	2:A:450:TRP:HD1	1.85	0.60
2:A:464:TYR:HA	2:A:500:ILE:HD12	1.84	0.60
2:A:525:LEU:HD13	2:A:527:VAL:HG12	1.84	0.60
2:A:211:ILE:HD12	2:A:232:ALA:CB	2.31	0.60
2:B:384:ILE:CD1	2:B:414:VAL:HG11	2.31	0.60
2:A:327:GLY:HA3	3:A:1001:SEP:HB2	1.84	0.60
2:A:381:ALA:O	2:A:385:VAL:HG23	2.02	0.60
2:B:347:VAL:HG13	2:B:348:TYR:CD2	2.36	0.60
2:B:497:LEU:O	2:B:500:ILE:HG22	2.02	0.60
2:A:49:LEU:O	2:A:53:ILE:HG12	2.02	0.59
2:A:463:ARG:HB2	2:A:466:ASP:OD2	2.02	0.59
2:A:144:ASP:HA	2:A:147:TYR:CE1	2.37	0.59
2:A:430:TYR:O	2:A:465:ILE:HG23	2.02	0.59
2:B:497:LEU:HA	2:B:500:ILE:HG22	1.84	0.59
2:A:19:ALA:O	2:A:22:ALA:HB3	2.03	0.59
2:A:53:ILE:HD13	2:A:330:VAL:HG11	1.84	0.59
2:A:434:VAL:HA	2:A:442:TYR:O	2.03	0.59
2:B:447:THR:C	2:B:449:LYS:H	2.06	0.59
2:B:101:PRO:HD3	2:B:177:ILE:HG12	1.84	0.59
2:B:533:ILE:HD13	2:B:533:ILE:N	2.17	0.59
2:B:286:HIS:CD2	2:B:288:LYS:H	2.20	0.59
2:B:367:LYS:HG3	2:B:503:TYR:CE1	2.38	0.59
1:D:968:U:H2'	1:D:969:G:H8	1.65	0.59
2:A:186:HIS:CD2	2:A:188:THR:HB	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:213:ARG:HH21	2:A:228:THR:HG21	1.68	0.59
2:A:53:ILE:O	2:A:57:ARG:HG3	2.03	0.58
2:A:413:ARG:HG3	2:A:532:GLU:HB2	1.83	0.58
2:B:494:VAL:O	2:B:522:ARG:HA	2.01	0.58
1:D:909:G:H5'	1:D:910:G:OP2	2.02	0.58
2:A:53:ILE:CD1	2:A:330:VAL:HG11	2.33	0.58
2:A:110:GLU:HG2	2:A:114:GLN:NE2	2.18	0.58
2:A:475:LYS:HE2	2:A:475:LYS:HA	1.84	0.58
1:D:942:C:HO2'	1:D:943:U:H5'	1.67	0.58
2:A:201:LYS:O	2:B:511:TYR:HB2	2.03	0.58
2:A:261:ASN:HD22	2:A:262:PHE:H	1.51	0.58
2:A:258:GLY:HA3	2:A:286:HIS:HE1	1.67	0.58
2:B:381:ALA:HA	2:B:384:ILE:CG1	2.33	0.58
2:A:397:PRO:HD3	2:A:421:GLU:CG	2.31	0.58
2:A:326:LEU:HD13	2:A:327:GLY:N	2.19	0.58
2:A:366:ILE:HA	2:A:504:ILE:HG22	1.84	0.58
2:A:428:PRO:HG2	2:A:524:PRO:HG2	1.85	0.58
2:B:363:ALA:HB2	2:B:458:VAL:HG21	1.86	0.58
2:A:306:PHE:HB2	2:A:324:MET:CE	2.34	0.58
2:A:310:SER:C	2:A:312:THR:H	2.06	0.58
2:B:381:ALA:HB2	2:B:473:ALA:CB	2.34	0.58
2:A:309:TYR:HD1	2:A:323:VAL:HG13	1.68	0.57
2:A:16:PHE:O	2:A:19:ALA:N	2.37	0.57
2:B:464:TYR:CA	2:B:500:ILE:HD11	2.32	0.57
2:B:525:LEU:HD22	2:B:527:VAL:HB	1.85	0.57
2:A:259:PHE:CD2	2:A:286:HIS:HB2	2.39	0.57
2:B:422:ASN:O	2:B:423:THR:HB	2.05	0.57
2:A:442:TYR:CE2	2:A:453:PHE:HE2	2.21	0.57
2:B:280:THR:HG22	2:B:281:GLU:N	2.20	0.57
2:B:343:VAL:HG12	2:B:344:ARG:N	2.20	0.57
2:A:162:LYS:O	2:A:166:GLU:HG2	2.05	0.56
2:A:381:ALA:HB2	2:A:473:ALA:CB	2.28	0.56
2:A:85:ARG:N	2:A:85:ARG:HD2	2.20	0.56
2:A:464:TYR:HA	2:A:500:ILE:CD1	2.35	0.56
2:A:471:TYR:HB2	2:A:501:ASN:ND2	2.21	0.56
2:B:72:LEU:HD21	2:B:215:PHE:HE1	1.70	0.56
2:A:23:GLY:O	2:A:25:GLU:N	2.37	0.56
2:A:211:ILE:HD12	2:A:232:ALA:HB1	1.87	0.56
2:A:215:PHE:CD1	2:A:215:PHE:N	2.71	0.56
2:A:292:SER:C	2:A:294:THR:H	2.09	0.56
2:A:444:ILE:HB	2:A:450:TRP:NE1	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:LEU:HD21	2:B:344:ARG:HG2	1.87	0.56
2:B:343:VAL:CG1	2:B:344:ARG:N	2.69	0.56
2:B:367:LYS:NZ	2:B:367:LYS:HB3	2.20	0.56
2:A:135:TYR:HA	2:A:139:GLU:HG3	1.88	0.56
2:B:80:LYS:HA	2:B:87:ALA:HB1	1.88	0.56
2:B:83:PHE:CE2	2:B:90:VAL:HG21	2.40	0.56
2:B:204:LEU:HD23	2:B:238:ASP:HA	1.87	0.56
2:B:401:LEU:HD11	2:B:413:ARG:HB3	1.88	0.56
2:A:350:GLN:NE2	2:B:68:VAL:HG23	2.21	0.56
2:A:434:VAL:O	2:A:460:THR:HG22	2.06	0.56
2:A:496:ASN:C	2:A:496:ASN:HD22	2.08	0.56
2:B:263:ARG:HG2	2:B:300:TRP:CH2	2.40	0.56
2:A:91:LEU:HD12	2:A:91:LEU:N	2.19	0.56
2:A:430:TYR:HB2	2:A:465:ILE:CG2	2.36	0.56
2:A:490:LYS:HB3	2:A:528:THR:CG2	2.36	0.56
2:B:68:VAL:O	2:B:210:SER:HB2	2.06	0.56
2:B:505:HIS:O	2:B:508:VAL:HG22	2.06	0.56
2:A:309:TYR:HD1	2:A:323:VAL:CG1	2.19	0.56
2:B:314:LEU:HD12	2:B:319:ILE:HB	1.86	0.55
2:A:441:ILE:HB	2:A:519:ILE:HD12	1.88	0.55
2:A:504:ILE:HB	2:A:508:VAL:CG2	2.36	0.55
1:D:903:C:H2'	1:D:904:A:O4'	2.05	0.55
1:D:956:G:O2'	1:D:957:A:H5'	2.05	0.55
2:A:533:ILE:H	2:A:533:ILE:CD1	2.09	0.55
2:B:514:TRP:C	2:B:516:LYS:H	2.10	0.55
1:D:934:U:H5''	1:D:935:A:O5'	2.06	0.55
2:A:166:GLU:HG3	2:A:167:VAL:HG23	1.89	0.55
2:A:290:VAL:HG23	2:A:290:VAL:O	2.07	0.55
2:B:102:LYS:NZ	2:B:102:LYS:HB3	2.21	0.55
2:B:261:ASN:HD22	2:B:262:PHE:H	1.54	0.55
2:B:331:GLU:O	2:B:335:MET:HG3	2.07	0.55
2:A:154:ASP:OD1	2:A:159:THR:HG21	2.06	0.55
2:A:410:ARG:O	2:A:412:VAL:HG23	2.06	0.55
2:B:397:PRO:HG3	2:B:420:ASN:O	2.07	0.55
1:D:936:G:O6	2:A:450:TRP:HZ2	1.90	0.55
2:A:156:ASP:CG	2:A:157:ASP:H	2.10	0.55
2:B:4:ASP:CG	2:B:7:LYS:HD3	2.27	0.55
2:A:401:LEU:HA	2:A:415:TYR:HD1	1.72	0.55
2:A:412:VAL:HG13	2:A:533:ILE:HG22	1.88	0.55
2:A:440:ASP:HB3	2:A:518:LYS:O	2.07	0.55
2:A:510:ARG:NH2	2:B:200:ASP:HB2	2.19	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:292:SER:HB3	2:A:294:THR:HG22	1.87	0.54
2:A:448:LYS:N	2:A:448:LYS:HD3	2.22	0.54
2:A:507:ASN:ND2	2:B:200:ASP:HA	2.21	0.54
1:D:912:A:H2'	1:D:913:G:O4'	2.07	0.54
2:B:91:LEU:HD22	2:B:96:TYR:OH	2.07	0.54
2:B:485:GLU:HA	2:B:533:ILE:O	2.06	0.54
2:A:301:ILE:HD11	2:A:332:ARG:CD	2.33	0.54
2:A:435:VAL:HG12	2:A:459:PRO:HA	1.88	0.54
1:D:943:U:C2'	1:D:944:U:H5'	2.36	0.54
2:A:31:SER:CB	2:A:32:PRO:CD	2.85	0.54
2:B:183:LEU:HB3	2:B:215:PHE:CD1	2.43	0.54
2:A:90:VAL:O	2:A:93:ARG:HG2	2.07	0.54
2:A:444:ILE:HD12	2:A:450:TRP:CG	2.43	0.54
2:A:533:ILE:O	2:A:533:ILE:HG12	2.08	0.54
2:A:391:HIS:HB3	2:A:394:GLU:HG3	1.89	0.54
2:B:53:ILE:HG23	2:B:211:ILE:CG2	2.37	0.54
2:A:351:ILE:HG22	2:A:352:HIS:CD2	2.36	0.53
2:A:465:ILE:HG13	2:A:466:ASP:N	2.23	0.53
2:B:260:GLU:OE2	2:B:287:PRO:HG3	2.07	0.53
2:A:16:PHE:O	2:A:18:ALA:N	2.41	0.53
2:A:250:ALA:O	2:A:254:LEU:HD23	2.07	0.53
2:A:145:LEU:HD22	2:A:145:LEU:N	2.23	0.53
2:A:183:LEU:HD11	2:B:183:LEU:HD11	1.89	0.53
2:B:209:PHE:HA	2:B:234:CYS:HA	1.89	0.53
2:B:474:ARG:HG3	2:B:474:ARG:HH11	1.73	0.53
2:A:47:HIS:CD2	2:A:49:LEU:HB2	2.43	0.53
2:B:80:LYS:HA	2:B:87:ALA:CB	2.39	0.53
2:B:492:ARG:HA	2:B:526:PHE:HD2	1.74	0.53
2:B:371:VAL:HG23	2:B:372:PRO:HD2	1.89	0.53
2:A:178:SER:CB	2:B:176:PRO:HB2	2.35	0.53
2:A:254:LEU:HD11	2:A:303:ILE:HG21	1.91	0.53
2:A:301:ILE:CD1	2:A:332:ARG:HD3	2.31	0.53
2:A:306:PHE:HB2	2:A:324:MET:HE1	1.89	0.53
2:A:31:SER:HB2	2:A:32:PRO:CD	2.39	0.53
2:A:104:ASN:HA	2:A:136:LYS:NZ	2.24	0.53
2:A:397:PRO:O	2:A:398:CYS:HB3	2.09	0.53
2:A:285:PHE:HB2	2:A:300:TRP:CD2	2.44	0.53
2:A:331:GLU:O	2:A:335:MET:HG3	2.09	0.53
2:B:398:CYS:O	2:B:417:VAL:HG23	2.09	0.53
2:B:504:ILE:HD11	2:B:509:ARG:NH2	2.23	0.52
2:A:30:ARG:HB3	2:A:34:GLU:HB3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:38:ARG:HH22	2:A:462:ILE:HD11	1.72	0.52
2:A:309:TYR:CD1	2:A:323:VAL:HG13	2.43	0.52
2:B:325:ASN:HD22	2:B:326:LEU:N	2.05	0.52
1:D:955:C:H2'	1:D:956:G:C8	2.44	0.52
2:B:342:ASP:HB3	2:B:345:LYS:HB2	1.91	0.52
2:B:403:PHE:HB3	2:B:414:VAL:HG23	1.91	0.52
2:A:95:PHE:CD2	2:B:97:LEU:HG	2.45	0.52
2:A:500:ILE:HG23	2:A:500:ILE:O	2.09	0.52
2:A:511:TYR:CE1	2:A:515:LYS:HG3	2.44	0.52
2:B:217:ARG:O	2:B:220:GLY:N	2.42	0.52
2:A:82:GLN:HG2	2:A:192:PHE:CE1	2.45	0.52
2:A:185:SER:HB2	2:A:216:ARG:HD3	1.91	0.52
2:A:198:ILE:HD13	2:A:202:LEU:HD12	1.91	0.52
2:B:381:ALA:HB1	2:B:469:ALA:CB	2.35	0.52
2:A:320:PRO:HG2	2:A:321:TYR:CD1	2.44	0.52
2:A:366:ILE:HD11	2:A:441:ILE:HD13	1.91	0.52
2:B:14:LYS:HD2	2:B:14:LYS:N	2.24	0.52
2:A:85:ARG:C	2:A:87:ALA:H	2.12	0.52
2:A:267:ASP:CB	2:A:279:GLN:HG2	2.39	0.52
2:A:464:TYR:CB	2:A:500:ILE:HD11	2.40	0.52
2:B:32:PRO:HD2	2:B:371:VAL:HG21	1.92	0.52
2:B:314:LEU:HD12	2:B:319:ILE:CB	2.40	0.51
2:B:533:ILE:O	2:B:533:ILE:HG12	2.08	0.51
2:A:310:SER:C	2:A:312:THR:N	2.63	0.51
2:A:32:PRO:HG3	2:A:371:VAL:CG2	2.39	0.51
2:A:188:THR:HG23	2:A:309:TYR:CZ	2.46	0.51
2:A:504:ILE:HD12	2:A:508:VAL:HG23	1.91	0.51
2:B:352:HIS:O	2:B:354:GLU:N	2.44	0.51
2:B:504:ILE:HD13	2:B:504:ILE:H	1.75	0.51
2:A:511:TYR:CZ	2:A:515:LYS:HG3	2.46	0.51
2:A:527:VAL:O	2:A:527:VAL:HG13	2.10	0.51
2:B:37:PRO:O	2:B:364:ARG:HA	2.10	0.51
2:B:464:TYR:O	2:B:500:ILE:HD11	2.11	0.51
1:D:918:G:O2'	1:D:919:C:OP1	2.25	0.51
2:A:31:SER:HB2	2:A:32:PRO:HD2	1.91	0.51
2:A:200:ASP:HA	2:B:507:ASN:HD22	1.76	0.51
2:A:258:GLY:O	2:A:259:PHE:C	2.49	0.51
2:B:271:SER:HB3	2:B:273:TYR:CE1	2.46	0.51
2:B:428:PRO:HG2	2:B:524:PRO:HG2	1.93	0.51
2:A:391:HIS:O	2:A:425:LEU:HD23	2.11	0.51
2:B:485:GLU:OE1	2:B:486:GLU:N	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:ASP:HB2	2:B:91:LEU:HD21	1.91	0.51
2:A:440:ASP:HB3	2:A:518:LYS:HG3	1.92	0.50
2:B:4:ASP:HB3	2:B:7:LYS:HB2	1.93	0.50
2:B:292:SER:OG	2:B:294:THR:HG22	2.11	0.50
2:A:145:LEU:HD22	2:A:145:LEU:H	1.77	0.50
2:A:153:LEU:O	2:A:154:ASP:HB2	2.10	0.50
2:A:500:ILE:HG21	2:A:502:LEU:HD22	1.94	0.50
2:A:306:PHE:CD1	2:A:306:PHE:C	2.84	0.50
2:B:430:TYR:HD2	2:B:465:ILE:HG21	1.75	0.50
2:B:264:PHE:HB3	2:B:280:THR:HG21	1.93	0.50
2:B:72:LEU:HA	2:B:184:ARG:HH21	1.77	0.50
2:B:385:VAL:O	2:B:389:GLU:HG3	2.12	0.50
2:B:412:VAL:CG2	2:B:533:ILE:HG22	2.39	0.50
2:B:85:ARG:HD2	2:B:85:ARG:N	2.26	0.50
2:B:364:ARG:HH21	2:B:364:ARG:HG3	1.77	0.50
2:A:261:ASN:HD22	2:A:262:PHE:N	2.10	0.50
2:B:283:PHE:CZ	2:B:302:GLU:HB2	2.47	0.50
2:A:155:VAL:HG22	2:A:158:ILE:HD13	1.94	0.50
2:A:197:HIS:NE2	2:B:351:ILE:HG23	2.27	0.50
2:A:500:ILE:HG22	2:A:502:LEU:HB2	1.94	0.50
2:B:463:ARG:NH1	2:B:465:ILE:HD11	2.26	0.50
1:D:907:G:C6	1:D:948:C:N4	2.80	0.49
2:B:5:PRO:O	2:B:9:ARG:HB2	2.11	0.49
2:B:270:ARG:O	2:B:271:SER:C	2.50	0.49
2:B:401:LEU:HD12	2:B:414:VAL:O	2.11	0.49
2:B:451:ARG:O	2:B:454:PHE:N	2.45	0.49
2:A:57:ARG:C	2:A:61:LEU:HD12	2.33	0.49
2:A:464:TYR:HB3	2:A:500:ILE:HD11	1.93	0.49
2:B:283:PHE:CE1	2:B:302:GLU:HB2	2.47	0.49
2:B:363:ALA:HB2	2:B:458:VAL:HG23	1.93	0.49
2:A:493:ILE:HG23	2:A:526:PHE:CE1	2.47	0.49
2:B:55:ARG:HG2	2:B:257:PHE:CE1	2.47	0.49
2:B:493:ILE:H	2:B:493:ILE:CD1	2.25	0.49
2:A:149:ILE:HD12	2:A:156:ASP:H	1.77	0.49
2:A:233:SER:HB2	3:A:1001:SEP:O3P	2.12	0.49
2:A:446:LYS:NZ	2:A:446:LYS:HB3	2.27	0.49
2:B:391:HIS:C	2:B:393:SER:H	2.15	0.49
2:B:504:ILE:HB	2:B:508:VAL:CG2	2.40	0.49
2:A:484:GLN:NE2	2:A:486:GLU:O	2.40	0.49
2:A:275:ILE:HG13	2:A:310:SER:HA	1.93	0.49
2:A:505:HIS:CE1	2:A:506:GLU:HG2	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:371:VAL:CG2	2:B:372:PRO:HD2	2.42	0.49
2:A:31:SER:CB	2:A:32:PRO:HD2	2.42	0.49
2:A:60:TYR:O	2:A:63:ILE:HG12	2.13	0.49
2:A:478:GLU:HA	2:A:481:MET:CE	2.43	0.49
2:A:478:GLU:HA	2:A:481:MET:HE2	1.93	0.49
2:B:254:LEU:HG	2:B:259:PHE:CD1	2.48	0.49
2:A:65:PHE:CD1	2:A:65:PHE:N	2.79	0.49
2:B:356:LYS:HG3	2:B:357:LEU:N	2.28	0.49
2:A:184:ARG:NH2	2:A:187:MET:SD	2.86	0.48
2:A:203:PRO:HG3	2:B:508:VAL:HG12	1.95	0.48
2:A:313:ALA:O	2:A:316:GLU:HB2	2.13	0.48
2:A:487:VAL:HG23	2:A:533:ILE:HD11	1.95	0.48
2:B:56:LEU:HB3	2:B:211:ILE:HD13	1.94	0.48
2:B:75:GLU:OE2	2:B:75:GLU:HA	2.13	0.48
2:A:401:LEU:HA	2:A:415:TYR:CD1	2.49	0.48
2:B:352:HIS:O	2:B:354:GLU:HG2	2.12	0.48
2:A:397:PRO:CD	2:A:421:GLU:HG2	2.35	0.48
2:B:220:GLY:HA2	2:B:227:TYR:HE2	1.78	0.48
2:B:301:ILE:HD11	2:B:332:ARG:HD3	1.95	0.48
2:B:355:ILE:O	2:B:355:ILE:HG13	2.12	0.48
2:A:500:ILE:O	2:A:500:ILE:CG2	2.61	0.48
1:D:916:G:H2'	1:D:959:U:O2'	2.13	0.48
2:A:213:ARG:HH21	2:A:228:THR:HG22	1.77	0.48
2:A:466:ASP:O	2:A:470:TYR:CD2	2.66	0.48
2:B:286:HIS:HD2	2:B:288:LYS:H	1.62	0.48
2:B:380:ILE:HG12	2:B:403:PHE:CE1	2.49	0.48
2:A:91:LEU:H	2:A:91:LEU:CD1	2.25	0.48
2:B:304:ALA:HB2	2:B:328:LEU:HD22	1.96	0.48
2:A:76:ASP:HB2	2:A:91:LEU:CD2	2.43	0.48
2:A:97:LEU:HD23	2:B:95:PHE:HE2	1.77	0.48
2:A:185:SER:HA	2:A:215:PHE:O	2.13	0.48
2:B:460:THR:HG22	2:B:462:ILE:HG12	1.96	0.48
2:A:32:PRO:HG3	2:A:371:VAL:HG22	1.96	0.48
2:A:56:LEU:HD13	2:A:257:PHE:CZ	2.48	0.48
2:A:275:ILE:HG23	2:A:276:PRO:CD	2.42	0.48
2:A:386:GLU:O	2:A:390:LYS:HG3	2.13	0.47
2:B:37:PRO:O	2:B:364:ARG:HG3	2.14	0.47
2:B:54:GLN:OE1	2:B:57:ARG:HD3	2.14	0.47
1:D:957:A:N3	1:D:959:U:C5	2.82	0.47
2:A:45:LYS:HB2	2:A:45:LYS:NZ	2.28	0.47
2:A:128:LEU:HB2	2:A:131:ILE:HB	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:74:VAL:HG21	2:A:189:THR:CG2	2.44	0.47
2:A:243:VAL:HG12	2:A:247:LYS:HE3	1.97	0.47
2:A:376:VAL:HG12	2:A:380:ILE:HD13	1.96	0.47
2:A:492:ARG:HG3	2:A:492:ARG:NH1	2.30	0.47
2:B:174:LEU:C	2:B:175:LYS:HD2	2.35	0.47
2:B:267:ASP:CB	2:B:279:GLN:HG2	2.30	0.47
2:B:437:TYR:CD2	2:B:438:LYS:HG2	2.49	0.47
1:D:957:A:O2'	1:D:958:A:P	2.72	0.47
2:A:332:ARG:O	2:A:335:MET:N	2.47	0.47
2:A:56:LEU:HD23	2:A:330:VAL:HG22	1.97	0.47
2:A:128:LEU:H	2:A:128:LEU:CD2	2.22	0.47
2:A:135:TYR:C	2:A:137:LYS:H	2.18	0.47
2:A:378:LEU:O	2:A:382:GLN:HB2	2.14	0.47
2:A:500:ILE:HG22	2:A:502:LEU:H	1.80	0.47
2:B:59:ALA:HA	2:B:256:GLN:OE1	2.15	0.47
2:B:75:GLU:CB	2:B:77:VAL:HG12	2.45	0.47
2:B:306:PHE:HB3	2:B:326:LEU:HD22	1.97	0.47
2:B:373:GLN:O	2:B:373:GLN:HG3	2.14	0.47
2:B:374:THR:O	2:B:378:LEU:HD23	2.15	0.47
2:B:380:ILE:HG12	2:B:403:PHE:CD1	2.50	0.47
1:D:939:C:H2'	1:D:940:C:C6	2.49	0.47
2:A:56:LEU:CD1	2:A:257:PHE:CZ	2.97	0.47
2:A:160:ALA:HA	2:A:163:ILE:CG2	2.45	0.47
2:A:407:MET:SD	2:A:477:GLU:HA	2.55	0.47
2:B:90:VAL:O	2:B:92:ASP:N	2.48	0.47
2:B:387:THR:HG21	2:B:402:ALA:HB2	1.96	0.47
2:B:211:ILE:HG12	2:B:232:ALA:HA	1.96	0.47
2:A:39:VAL:O	2:A:364:ARG:NH2	2.48	0.47
2:A:171:PHE:N	2:A:171:PHE:CD2	2.82	0.47
2:A:234:CYS:SG	2:A:326:LEU:HB3	2.54	0.46
2:A:434:VAL:HG21	2:A:502:LEU:HD23	1.97	0.46
2:B:218:GLU:OE2	2:B:218:GLU:HA	2.14	0.46
2:B:430:TYR:CD2	2:B:465:ILE:HD13	2.50	0.46
2:A:445:PRO:HD2	2:A:450:TRP:HE1	1.79	0.46
2:A:460:THR:HG23	2:A:462:ILE:N	2.22	0.46
2:B:263:ARG:O	2:B:283:PHE:HB2	2.15	0.46
2:B:303:ILE:HG13	2:B:303:ILE:O	2.15	0.46
2:B:440:ASP:HB2	2:B:442:TYR:CZ	2.51	0.46
1:D:908:U:HO2'	1:D:946:A:H2	1.62	0.46
1:D:909:G:H1'	1:D:946:A:H1'	1.98	0.46
2:A:30:ARG:HB3	2:A:34:GLU:CB	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:HIS:CD2	2:B:49:LEU:HB2	2.51	0.46
2:B:287:PRO:O	2:B:290:VAL:HG22	2.15	0.46
2:B:325:ASN:C	2:B:325:ASN:ND2	2.69	0.46
2:B:505:HIS:CD2	2:B:506:GLU:HG2	2.51	0.46
2:B:520:ASP:O	2:B:520:ASP:OD1	2.34	0.46
2:A:494:VAL:HG22	2:A:499:ASP:O	2.15	0.46
2:A:510:ARG:HE	2:B:200:ASP:HB2	1.81	0.46
2:B:39:VAL:HG23	2:B:39:VAL:O	2.15	0.46
2:B:325:ASN:HD22	2:B:325:ASN:C	2.18	0.46
2:B:360:LEU:O	2:B:363:ALA:HB3	2.16	0.46
2:B:496:ASN:HB2	2:B:497:LEU:HD12	1.96	0.46
2:A:90:VAL:O	2:A:92:ASP:N	2.49	0.46
2:A:407:MET:HG2	2:A:408:MET:HG3	1.97	0.46
2:A:458:VAL:O	2:A:458:VAL:CG2	2.64	0.46
2:B:340:TYR:CD2	2:B:346:MET:HA	2.50	0.46
2:B:420:ASN:HD22	2:B:420:ASN:N	2.13	0.46
2:B:430:TYR:HB2	2:B:465:ILE:CG2	2.46	0.46
2:B:504:ILE:HD13	2:B:504:ILE:N	2.30	0.46
2:B:511:TYR:O	2:B:512:ILE:C	2.54	0.46
2:A:488:LYS:HA	2:A:530:LYS:HA	1.97	0.46
2:A:508:VAL:O	2:A:512:ILE:HG12	2.16	0.46
2:B:187:MET:HG2	2:B:233:SER:HB3	1.98	0.46
2:A:34:GLU:C	2:A:35:LEU:HD12	2.36	0.45
2:A:370:GLU:N	2:A:501:ASN:OD1	2.46	0.45
2:B:282:VAL:HG23	2:B:303:ILE:HG22	1.98	0.45
2:A:16:PHE:O	2:A:17:GLU:C	2.55	0.45
2:A:188:THR:HA	2:A:191:TRP:HD1	1.81	0.45
2:B:493:ILE:N	2:B:493:ILE:HD13	2.32	0.45
1:D:942:C:C2'	1:D:943:U:H5'	2.46	0.45
2:A:223:ALA:CA	2:A:344:ARG:HD2	2.36	0.45
2:A:340:TYR:CG	2:A:346:MET:HG3	2.51	0.45
2:B:259:PHE:CD2	2:B:286:HIS:HB2	2.51	0.45
2:B:450:TRP:O	2:B:451:ARG:C	2.54	0.45
1:D:923:G:H2'	1:D:924:C:C6	2.52	0.45
2:A:310:SER:O	2:A:312:THR:N	2.49	0.45
2:A:368:VAL:HG12	2:A:371:VAL:HG23	1.98	0.45
2:A:489:VAL:O	2:A:528:THR:HG23	2.16	0.45
2:B:274:TYR:O	2:B:275:ILE:C	2.54	0.45
2:B:393:SER:O	2:B:394:GLU:C	2.55	0.45
2:B:421:GLU:OE1	2:B:421:GLU:N	2.49	0.45
2:A:35:LEU:HD12	2:A:35:LEU:N	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:115:ILE:HG12	2:A:115:ILE:O	2.16	0.45
2:A:166:GLU:HG3	2:A:167:VAL:N	2.31	0.45
2:A:500:ILE:CG2	2:A:502:LEU:HD22	2.47	0.45
2:B:32:PRO:O	2:B:35:LEU:HD12	2.16	0.45
2:A:346:MET:O	2:A:349:PRO:HD3	2.17	0.45
2:A:371:VAL:O	2:A:372:PRO:O	2.35	0.45
2:A:414:VAL:HG21	2:A:476:VAL:HG11	1.97	0.45
2:A:468:PHE:O	2:A:471:TYR:N	2.48	0.45
2:B:98:ALA:HB2	2:B:178:SER:HA	1.99	0.45
2:B:426:CYS:HA	2:B:527:VAL:HG22	1.98	0.45
2:B:472:ALA:O	2:B:475:LYS:N	2.49	0.45
2:A:137:LYS:HE3	2:A:137:LYS:HA	1.98	0.45
2:A:287:PRO:O	2:A:289:LEU:N	2.50	0.45
2:A:351:ILE:HA	2:B:197:HIS:ND1	2.32	0.45
2:A:374:THR:HG22	2:A:376:VAL:H	1.81	0.45
2:B:47:HIS:CG	2:B:48:PRO:HD2	2.52	0.45
2:A:92:ASP:O	2:A:217:ARG:NH2	2.50	0.45
2:A:157:ASP:HB3	2:A:161:VAL:HG13	1.98	0.45
2:B:429:ALA:O	2:B:464:TYR:CD2	2.70	0.45
2:B:463:ARG:HB2	2:B:466:ASP:OD2	2.16	0.45
2:A:71:PRO:HG2	2:A:193:ILE:HG21	1.99	0.44
2:A:377:GLY:HA3	2:A:477:GLU:OE1	2.18	0.44
2:A:486:GLU:HG3	2:A:532:GLU:OE2	2.17	0.44
2:B:275:ILE:HG12	2:B:311:PRO:HD3	1.98	0.44
2:B:430:TYR:HB2	2:B:465:ILE:HG23	1.99	0.44
2:A:56:LEU:HD12	2:A:56:LEU:HA	1.78	0.44
2:A:117:ALA:O	2:A:118:ILE:C	2.54	0.44
2:A:395:PRO:HA	2:A:423:THR:O	2.17	0.44
2:A:413:ARG:NH1	2:A:532:GLU:HG3	2.33	0.44
2:B:192:PHE:HB3	2:B:317:TYR:CD1	2.52	0.44
2:B:513:LEU:O	2:B:516:LYS:N	2.50	0.44
2:A:213:ARG:NH2	2:A:228:THR:CG2	2.77	0.44
2:A:468:PHE:CD1	2:A:468:PHE:C	2.91	0.44
2:A:484:GLN:NE2	2:A:486:GLU:H	2.15	0.44
2:B:196:SER:HA	2:B:319:ILE:CD1	2.44	0.44
2:A:387:THR:HG21	2:A:402:ALA:HA	2.00	0.44
2:A:463:ARG:H	2:A:466:ASP:HB2	1.81	0.44
2:B:392:ALA:CB	2:B:426:CYS:HB2	2.44	0.44
2:A:450:TRP:HA	2:A:450:TRP:CE3	2.52	0.44
2:B:21:LYS:HB2	2:B:21:LYS:NZ	2.32	0.44
2:B:354:GLU:OE2	2:B:354:GLU:HA	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:909:G:C5'	1:D:910:G:OP2	2.66	0.44
2:A:355:ILE:O	2:A:515:LYS:CE	2.66	0.44
2:B:47:HIS:CD2	2:B:48:PRO:HD2	2.52	0.44
2:B:72:LEU:O	2:B:72:LEU:HD23	2.18	0.44
2:A:103:PRO:O	2:A:105:VAL:N	2.51	0.44
2:A:134:ARG:O	2:A:139:GLU:HG2	2.18	0.44
2:A:342:ASP:O	2:A:343:VAL:C	2.56	0.44
2:A:500:ILE:O	2:A:501:ASN:CB	2.66	0.44
2:B:74:VAL:HG21	2:B:189:THR:HG21	1.98	0.44
2:B:447:THR:C	2:B:449:LYS:N	2.71	0.44
2:A:95:PHE:HE1	2:A:216:ARG:O	2.01	0.44
2:A:359:ASP:HB3	2:A:458:VAL:HG13	2.00	0.44
2:A:475:LYS:HE2	2:A:475:LYS:CA	2.48	0.44
2:B:255:ARG:C	2:B:257:PHE:H	2.22	0.44
2:B:352:HIS:C	2:B:354:GLU:H	2.21	0.44
2:B:410:ARG:HD3	2:B:410:ARG:N	2.32	0.44
2:B:440:ASP:OD1	2:B:518:LYS:N	2.46	0.44
2:B:497:LEU:O	2:B:500:ILE:N	2.46	0.44
2:A:496:ASN:ND2	2:A:498:SER:HB3	2.32	0.44
2:A:515:LYS:O	2:A:516:LYS:HB2	2.18	0.44
2:B:32:PRO:O	2:B:38:ARG:NH1	2.51	0.44
2:B:198:ILE:HB	2:B:202:LEU:CD1	2.48	0.44
2:B:468:PHE:O	2:B:469:ALA:C	2.55	0.44
2:A:33:ASN:OD1	2:A:38:ARG:HD3	2.18	0.43
2:A:195:LEU:HD22	2:A:237:VAL:HG21	2.00	0.43
2:A:475:LYS:O	2:A:478:GLU:HB2	2.17	0.43
2:B:6:GLN:O	2:B:7:LYS:C	2.57	0.43
2:A:106:GLY:HA2	2:A:110:GLU:HB2	2.00	0.43
2:A:135:TYR:HA	2:A:139:GLU:HG2	2.00	0.43
2:A:23:GLY:C	2:A:25:GLU:N	2.72	0.43
2:A:55:ARG:HB3	2:A:55:ARG:HH21	1.82	0.43
2:B:275:ILE:HG13	2:B:310:SER:HA	2.01	0.43
2:B:415:TYR:O	2:B:529:VAL:HG13	2.18	0.43
2:A:47:HIS:ND1	2:A:48:PRO:HD2	2.33	0.43
2:A:65:PHE:CD2	2:A:234:CYS:HB2	2.52	0.43
2:A:347:VAL:HG13	2:A:348:TYR:CD2	2.53	0.43
2:B:185:SER:HA	2:B:215:PHE:O	2.18	0.43
2:B:347:VAL:HG13	2:B:348:TYR:HD2	1.83	0.43
1:D:908:U:H4'	1:D:947:C:O4'	2.19	0.43
2:A:95:PHE:HD2	2:B:97:LEU:HG	1.82	0.43
2:A:447:THR:CG2	2:A:448:LYS:N	2.81	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:500:ILE:HG13	2:B:500:ILE:O	2.19	0.43
1:D:925:G:H2'	1:D:926:G:H8	1.79	0.43
2:A:309:TYR:HB3	2:A:314:LEU:HD13	2.01	0.43
2:A:399:SER:HA	2:A:417:VAL:HG12	2.00	0.43
2:A:131:ILE:HD12	2:A:131:ILE:N	2.34	0.43
2:A:184:ARG:HH12	2:A:212:ASP:HB3	1.84	0.43
2:A:265:ARG:HG2	2:A:281:GLU:HB2	2.01	0.43
2:A:463:ARG:O	2:A:464:TYR:C	2.58	0.43
2:B:223:ALA:HA	2:B:344:ARG:NH2	2.34	0.43
2:B:381:ALA:CA	2:B:384:ILE:HG12	2.47	0.43
2:B:458:VAL:HA	2:B:459:PRO:HD2	1.91	0.43
2:A:67:GLU:CD	2:B:50:PHE:HD1	2.22	0.43
2:A:107:ILE:HG22	2:A:108:SER:N	2.33	0.43
2:A:371:VAL:HG13	2:A:372:PRO:HD2	2.01	0.43
2:A:376:VAL:HG11	2:A:407:MET:HB2	2.00	0.43
2:A:67:GLU:OE1	2:B:50:PHE:CD1	2.72	0.42
2:A:110:GLU:O	2:A:113:ARG:HB3	2.19	0.42
2:A:133:HIS:C	2:A:135:TYR:H	2.23	0.42
2:A:215:PHE:N	2:A:215:PHE:HD1	2.16	0.42
2:A:370:GLU:HB2	2:A:501:ASN:HD21	1.83	0.42
2:A:432:ASN:ND2	2:A:445:PRO:HD3	2.34	0.42
2:A:496:ASN:HD21	2:A:498:SER:HB3	1.84	0.42
2:B:73:ILE:HG21	2:B:181:LEU:HD13	2.01	0.42
2:A:155:VAL:O	2:A:156:ASP:C	2.57	0.42
2:A:166:GLU:HG3	2:A:167:VAL:H	1.84	0.42
2:A:353:GLY:HA3	2:A:514:TRP:HZ2	1.84	0.42
2:A:398:CYS:HG	2:A:400:PHE:HE2	1.60	0.42
1:D:917:G:O2'	1:D:918:G:O5'	2.36	0.42
2:A:458:VAL:O	2:A:458:VAL:HG22	2.18	0.42
2:A:528:THR:HG22	2:A:529:VAL:N	2.34	0.42
2:B:282:VAL:CG2	2:B:304:ALA:HB3	2.49	0.42
2:B:488:LYS:HD3	2:B:530:LYS:HE2	2.02	0.42
2:A:188:THR:HG23	2:A:309:TYR:CE2	2.54	0.42
2:A:340:TYR:CD1	2:A:346:MET:HG3	2.55	0.42
2:B:6:GLN:O	2:B:9:ARG:N	2.52	0.42
2:A:67:GLU:HB2	2:B:46:GLU:HA	2.01	0.42
2:B:504:ILE:HD11	2:B:509:ARG:CZ	2.49	0.42
1:D:923:G:O2'	1:D:924:C:H5'	2.19	0.42
2:A:3:PHE:CD1	2:A:3:PHE:C	2.93	0.42
2:A:23:GLY:C	2:A:25:GLU:H	2.22	0.42
2:A:285:PHE:CE2	2:A:299:GLY:HA3	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:ARG:HH11	2:B:212:ASP:HB3	1.85	0.42
2:B:314:LEU:HB3	2:B:319:ILE:HB	2.02	0.42
2:B:505:HIS:CD2	2:B:506:GLU:N	2.88	0.42
1:D:960:C:H6	1:D:960:C:O5'	2.02	0.42
2:A:65:PHE:N	2:A:65:PHE:HD1	2.18	0.42
2:A:104:ASN:HA	2:A:136:LYS:HZ2	1.84	0.42
2:A:383:SER:C	2:A:385:VAL:N	2.73	0.42
2:A:52:THR:O	2:A:56:LEU:HB2	2.19	0.42
2:A:314:LEU:HD21	2:A:323:VAL:HG12	2.00	0.42
2:B:294:THR:OG1	2:B:295:LYS:N	2.52	0.42
2:A:85:ARG:C	2:A:87:ALA:N	2.73	0.42
2:A:197:HIS:CD2	2:B:351:ILE:HA	2.54	0.42
2:A:347:VAL:HG13	2:A:348:TYR:N	2.34	0.42
2:B:285:PHE:CE2	2:B:299:GLY:HA3	2.55	0.42
2:B:497:LEU:CD1	2:B:509:ARG:HH12	2.29	0.42
2:A:45:LYS:NZ	2:A:45:LYS:CB	2.83	0.42
2:A:246:GLY:HA3	2:A:306:PHE:CE1	2.55	0.42
2:A:365:GLU:HG3	2:A:508:VAL:HG11	2.01	0.42
2:B:379:LYS:HA	2:B:382:GLN:HE21	1.85	0.42
2:B:490:LYS:HA	2:B:528:THR:HA	2.02	0.42
2:A:3:PHE:CD2	2:A:26:ILE:HG21	2.47	0.41
2:A:496:ASN:HD22	2:A:499:ASP:H	1.68	0.41
2:B:75:GLU:HB3	2:B:77:VAL:HG12	2.02	0.41
2:B:254:LEU:HD21	2:B:303:ILE:HG23	1.96	0.41
2:B:320:PRO:HG2	2:B:321:TYR:CD1	2.55	0.41
1:D:923:G:H2'	1:D:924:C:H6	1.86	0.41
2:A:218:GLU:O	2:A:219:GLN:O	2.38	0.41
2:A:396:SER:HB2	2:A:397:PRO:HA	2.02	0.41
2:A:500:ILE:HA	2:A:500:ILE:HD13	1.70	0.41
2:B:174:LEU:CB	2:B:175:LYS:HD2	2.50	0.41
2:B:442:TYR:CE2	2:B:453:PHE:CE2	3.08	0.41
2:B:464:TYR:HA	2:B:500:ILE:CD1	2.40	0.41
2:A:31:SER:O	2:A:35:LEU:HD13	2.19	0.41
2:A:65:PHE:HD1	2:A:65:PHE:H	1.68	0.41
2:A:90:VAL:HG13	2:A:93:ARG:HE	1.84	0.41
2:A:410:ARG:NH1	2:A:534:GLU:OXT	2.54	0.41
2:A:533:ILE:HD13	2:A:533:ILE:N	2.16	0.41
2:B:482:ARG:HD2	2:B:484:GLN:HE21	1.85	0.41
2:B:490:LYS:HB3	2:B:528:THR:HG23	2.03	0.41
2:B:519:ILE:HG22	2:B:521:VAL:HG23	2.02	0.41
1:D:919:C:H6	1:D:919:C:O5'	2.04	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:100:LEU:HD21	2:A:176:PRO:HD3	2.02	0.41
2:B:198:ILE:HB	2:B:202:LEU:HD12	2.03	0.41
2:A:486:GLU:CD	2:A:488:LYS:HE3	2.40	0.41
2:B:261:ASN:HD22	2:B:262:PHE:N	2.17	0.41
2:B:290:VAL:HG23	2:B:290:VAL:O	2.20	0.41
2:B:412:VAL:HG12	2:B:413:ARG:N	2.34	0.41
2:B:482:ARG:O	2:B:483:GLU:HB2	2.20	0.41
2:A:366:ILE:CD1	2:A:441:ILE:HD13	2.50	0.41
2:A:430:TYR:HD2	2:A:465:ILE:HG21	1.84	0.41
2:B:373:GLN:HB3	2:B:477:GLU:OE2	2.21	0.41
2:B:318:ASP:O	2:B:320:PRO:HD3	2.20	0.41
2:B:417:VAL:HG22	2:B:418:ASN:N	2.36	0.41
2:A:315:ALA:C	2:A:317:TYR:N	2.72	0.41
2:A:429:ALA:O	2:A:464:TYR:CD2	2.73	0.41
2:A:495:GLU:HA	2:A:522:ARG:HG2	2.02	0.41
2:B:217:ARG:O	2:B:218:GLU:C	2.58	0.41
2:B:326:LEU:HD13	2:B:327:GLY:N	2.35	0.41
1:D:935:A:C4	2:A:524:PRO:HD2	2.56	0.41
1:D:935:A:H1'	2:A:524:PRO:HD3	2.02	0.41
2:A:290:VAL:HA	2:A:297:SER:O	2.20	0.41
2:A:360:LEU:HA	2:A:458:VAL:HG21	2.02	0.41
2:A:444:ILE:HB	2:A:450:TRP:CD1	2.56	0.41
2:B:32:PRO:O	2:B:35:LEU:CD1	2.69	0.41
2:B:322:PRO:O	2:B:323:VAL:HG23	2.21	0.41
2:B:380:ILE:O	2:B:383:SER:OG	2.29	0.41
2:B:407:MET:O	2:B:408:MET:HB2	2.21	0.41
2:A:103:PRO:O	2:A:105:VAL:HG13	2.20	0.41
2:B:72:LEU:HD21	2:B:215:PHE:CE1	2.53	0.41
2:B:317:TYR:O	2:B:318:ASP:HB2	2.20	0.41
2:B:447:THR:O	2:B:449:LYS:N	2.54	0.41
2:A:493:ILE:HD12	2:A:493:ILE:O	2.20	0.40
2:A:505:HIS:ND1	2:A:506:GLU:N	2.69	0.40
2:B:83:PHE:CZ	2:B:90:VAL:HG21	2.56	0.40
2:B:102:LYS:HB3	2:B:102:LYS:HZ2	1.86	0.40
2:B:442:TYR:CE2	2:B:453:PHE:HE2	2.40	0.40
2:A:85:ARG:N	2:A:85:ARG:CD	2.84	0.40
2:A:464:TYR:N	2:A:464:TYR:CD1	2.89	0.40
2:B:493:ILE:CD1	2:B:493:ILE:N	2.84	0.40
2:A:149:ILE:HD12	2:A:156:ASP:N	2.36	0.40
2:A:442:TYR:CD1	2:A:520:ASP:HB3	2.56	0.40
2:B:241:LEU:HD12	2:B:322:PRO:HG2	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:340:TYR:CD2	2:B:346:MET:HB2	2.56	0.40
2:B:391:HIS:O	2:B:425:LEU:HD23	2.22	0.40
2:A:305:THR:HG22	2:A:306:PHE:N	2.37	0.40
2:A:394:GLU:O	2:A:396:SER:N	2.54	0.40
2:B:264:PHE:HD2	2:B:282:VAL:HA	1.86	0.40
2:A:184:ARG:NH1	2:A:212:ASP:OD2	2.55	0.40
2:A:385:VAL:O	2:A:389:GLU:N	2.47	0.40
2:A:452:SER:HG	2:A:453:PHE:HD1	1.67	0.40
2:B:218:GLU:C	2:B:220:GLY:H	2.25	0.40
2:B:374:THR:HG23	2:B:477:GLU:CD	2.42	0.40
2:B:494:VAL:HG23	2:B:523:GLY:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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
2	A	532/534 (100%)	387 (73%)	100 (19%)	45 (8%)	1 5
2	B	461/534 (86%)	372 (81%)	67 (14%)	22 (5%)	2 14
All	All	993/1068 (93%)	759 (76%)	167 (17%)	67 (7%)	1 8

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	31	SER
2	A	156	ASP
2	A	220	GLY
2	A	225	ARG
2	A	372	PRO
2	A	484	GLN
2	A	526	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	527	VAL
2	B	14	LYS
2	B	421	GLU
2	B	423	THR
2	B	484	GLN
2	B	516	LYS
2	A	17	GLU
2	A	24	LYS
2	A	104	ASN
2	A	107	ILE
2	A	118	ILE
2	A	140	ILE
2	A	219	GLN
2	A	259	PHE
2	A	343	VAL
2	A	485	GLU
2	A	500	ILE
2	B	218	GLU
2	B	353	GLY
2	B	451	ARG
2	A	32	PRO
2	A	91	LEU
2	A	121	ARG
2	A	125	SER
2	A	288	LYS
2	A	291	GLY
2	A	293	SER
2	A	369	LYS
2	A	395	PRO
2	A	398	CYS
2	A	420	ASN
2	B	91	LEU
2	B	352	HIS
2	B	363	ALA
2	B	364	ARG
2	B	438	LYS
2	B	448	LYS
2	A	84	GLY
2	A	86	GLU
2	A	115	ILE
2	A	127	PRO
2	A	148	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	153	LEU
2	A	154	ASP
2	A	171	PHE
2	A	483	GLU
2	B	24	LYS
2	B	223	ALA
2	B	256	GLN
2	B	420	ASN
2	B	469	ALA
2	A	20	TRP
2	B	496	ASN
2	B	394	GLU
2	B	409	GLY
2	A	105	VAL
2	A	339	GLY
2	A	138	GLY
2	A	152	VAL
2	A	290	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	
2	A	464/464 (100%)	430 (93%)	34 (7%)	14	41
2	B	402/464 (87%)	369 (92%)	33 (8%)	11	36
All	All	866/928 (93%)	799 (92%)	67 (8%)	13	38

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	8	TYR
2	A	49	LEU
2	A	55	ARG
2	A	56	LEU
2	A	61	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	65	PHE
2	A	68	VAL
2	A	77	VAL
2	A	85	ARG
2	A	104	ASN
2	A	147	TYR
2	A	165	ASP
2	A	186	HIS
2	A	215	PHE
2	A	255	ARG
2	A	261	ASN
2	A	301	ILE
2	A	314	LEU
2	A	324	MET
2	A	325	ASN
2	A	333	LEU
2	A	344	ARG
2	A	378	LEU
2	A	382	GLN
2	A	386	GLU
2	A	422	ASN
2	A	440	ASP
2	A	471	TYR
2	A	485	GLU
2	A	496	ASN
2	A	500	ILE
2	A	502	LEU
2	A	509	ARG
2	A	533	ILE
2	B	6	GLN
2	B	7	LYS
2	B	31	SER
2	B	35	LEU
2	B	38	ARG
2	B	49	LEU
2	B	55	ARG
2	B	85	ARG
2	B	97	LEU
2	B	180	THR
2	B	186	HIS
2	B	216	ARG
2	B	245	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	254	LEU
2	B	261	ASN
2	B	325	ASN
2	B	326	LEU
2	B	328	LEU
2	B	333	LEU
2	B	343	VAL
2	B	352	HIS
2	B	367	LYS
2	B	410	ARG
2	B	448	LYS
2	B	451	ARG
2	B	485	GLU
2	B	493	ILE
2	B	497	LEU
2	B	499	ASP
2	B	504	ILE
2	B	509	ARG
2	B	525	LEU
2	B	533	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	104	ASN
2	A	114	GLN
2	A	261	ASN
2	A	325	ASN
2	A	352	HIS
2	A	382	GLN
2	A	422	ASN
2	A	496	ASN
2	B	47	HIS
2	B	261	ASN
2	B	286	HIS
2	B	382	GLN
2	B	420	ASN
2	B	484	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	D	70/71 (98%)	17 (24%)	3 (4%)

All (17) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	D	906	G
1	D	908	U
1	D	909	G
1	D	910	G
1	D	917	G
1	D	918	G
1	D	919	C
1	D	932	U
1	D	933	C
1	D	935	A
1	D	943	U
1	D	944	U
1	D	945	U
1	D	946	A
1	D	958	A
1	D	960	C
1	D	968	U

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	D	917	G
1	D	934	U
1	D	957	A

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SEP	A	1001	-	9,10,10	1.56	1 (11%)	12,14,14	1.69	2 (16%)
3	SEP	A	1002	-	9,10,10	1.54	1 (11%)	12,14,14	1.85	2 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SEP	A	1001	-	-	6/10/10/10	-
3	SEP	A	1002	-	-	4/10/10/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	SEP	P-O1P	3.39	1.61	1.50
3	A	1001	SEP	P-O1P	3.37	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	SEP	OG-CB-CA	5.29	112.67	108.06
3	A	1001	SEP	OG-CB-CA	4.52	112.00	108.06
3	A	1001	SEP	O3P-P-OG	2.48	113.34	106.73
3	A	1002	SEP	O3P-P-OG	2.45	113.25	106.73

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	SEP	CA-CB-OG-P
3	A	1001	SEP	CB-OG-P-O2P
3	A	1001	SEP	CB-OG-P-O3P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	1002	SEP	CB-OG-P-O1P
3	A	1002	SEP	CB-OG-P-O2P
3	A	1002	SEP	CB-OG-P-O3P
3	A	1002	SEP	CA-CB-OG-P
3	A	1001	SEP	OXT-C-CA-CB
3	A	1001	SEP	CB-OG-P-O1P
3	A	1001	SEP	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	SEP	2	0
3	A	1002	SEP	1	0

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	D	71/71 (100%)	3.22	58 (81%) 0 0	112, 199, 201, 201	0
2	A	534/534 (100%)	0.43	43 (8%) 12 11	15, 79, 197, 201	0
2	B	465/534 (87%)	0.07	11 (2%) 59 56	9, 66, 175, 200	0
All	All	1070/1139 (93%)	0.46	112 (10%) 6 6	9, 77, 199, 201	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	969	G	8.1
1	D	970	G	7.7
1	D	933	C	6.4
2	A	108	SER	6.4
1	D	903	C	6.1
2	A	103	PRO	6.0
2	B	223	ALA	6.0
2	A	533	ILE	5.9
1	D	905	G	5.7
2	A	133	HIS	5.6
1	D	929	G	5.6
1	D	928	G	5.5
1	D	965	C	5.4
1	D	951	G	5.4
2	A	407	MET	5.3
1	D	971	C	5.2
1	D	957	A	5.2
1	D	941	G	5.1
1	D	901	G	5.0
2	A	422	ASN	5.0
1	D	940	C	4.9
1	D	939	C	4.9
1	D	902	C	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	106	GLY	4.3
1	D	925	G	4.3
1	D	904	A	4.3
1	D	952	G	4.3
2	A	107	ILE	4.0
2	A	173	GLU	3.7
1	D	942	C	3.7
1	D	930	A	3.7
1	D	906	G	3.7
2	B	222	ASP	3.7
2	A	116	GLU	3.7
1	D	968	U	3.6
2	A	151	GLU	3.6
1	D	966	C	3.6
1	D	936	G	3.6
2	A	117	ALA	3.6
2	A	149	ILE	3.6
1	D	931	C	3.5
2	B	488	LYS	3.5
1	D	945	U	3.5
2	B	468	PHE	3.5
2	A	132	PHE	3.5
1	D	958	A	3.4
2	A	152	VAL	3.4
1	D	924	C	3.4
1	D	915	G	3.4
2	A	150	ALA	3.3
2	A	534	GLU	3.3
2	A	131	ILE	3.2
2	B	529	VAL	3.2
1	D	964	G	3.2
2	B	42	SER	3.2
1	D	937	A	3.2
2	A	109	ALA	3.2
2	A	531	ALA	3.1
1	D	907	G	3.1
2	A	223	ALA	3.0
1	D	956	G	3.0
2	A	137	LYS	2.9
1	D	947	C	2.9
2	A	126	LYS	2.9
1	D	927	C	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	155	VAL	2.8
1	D	935	A	2.8
1	D	950	C	2.7
1	D	967	C	2.7
2	A	404	GLU	2.7
2	B	489	VAL	2.7
2	A	168	PHE	2.7
2	A	156	ASP	2.7
2	A	171	PHE	2.6
1	D	961	C	2.6
1	D	926	G	2.6
2	B	407	MET	2.6
2	B	422	ASN	2.6
2	A	411	ASN	2.6
1	D	963	G	2.5
1	D	943	U	2.5
1	D	932	U	2.5
2	A	403	PHE	2.5
2	A	487	VAL	2.5
1	D	959	U	2.4
1	D	910	G	2.4
1	D	913	G	2.4
2	A	476	VAL	2.4
1	D	923	G	2.4
1	D	944	U	2.3
1	D	922	U	2.3
1	D	953	U	2.3
2	A	120	LYS	2.3
1	D	917	G	2.2
2	A	224	THR	2.2
2	A	85	ARG	2.2
1	D	938	U	2.2
2	B	295	LYS	2.2
2	A	62	SER	2.2
2	A	110	GLU	2.1
2	A	412	VAL	2.1
1	D	934	U	2.1
1	D	948	C	2.1
1	D	960	C	2.1
1	D	954	U	2.0
2	B	487	VAL	2.0
1	D	949	C	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	123	VAL	2.0
2	A	161	VAL	2.0
2	A	163	ILE	2.0
2	A	174	LEU	2.0
2	A	105	VAL	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 monosaccharides 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(\AA^2)	Q<0.9
3	SEP	A	1001	11/11	0.93	0.29	55,90,119,121	0
3	SEP	A	1002	11/11	0.93	0.27	35,68,109,116	0

6.5 Other polymers [i](#)

There are no such residues in this entry.