



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:05 AM UTC

PDB ID : 2C4R / pdb_00002c4r
Title : Catalytic domain of E. coli RNase E
Authors : Marcaida, M.J.; Callaghan, A.J.; Luisi, B.F.
Deposited on : 2005-10-21
Resolution : 3.60 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

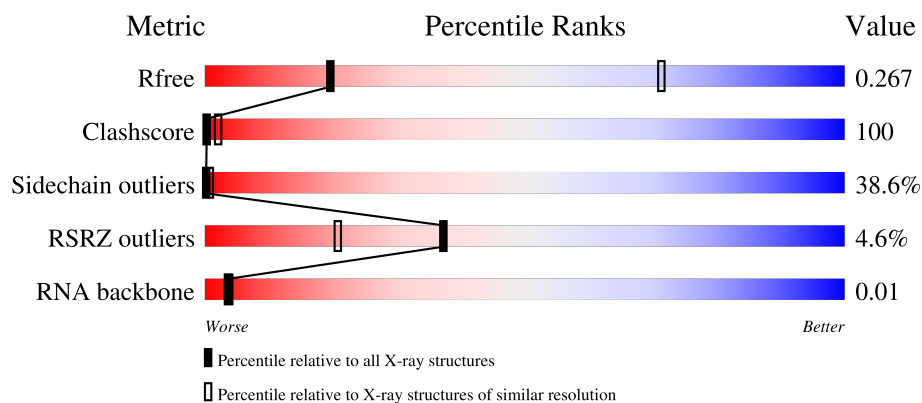
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)
RNA backbone	3983	1014 (4.14-3.06)

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	L	517	4% 19% 50% 23% • 5%
2	R	10	10% 20% 80%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3778 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 RIBONUCLEASE E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	491	Total	C	N	O	S	0	0	0
			3557	2223	649	674	11			

- Molecule 2 is a RNA chain called SSRNA MOLECULE: 5'-R(*AP*CP*AP*GP*UP*AP*UP*UP*GP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	10	Total	C	N	O	P	0	0	0
			212	95	36	71	10			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	2	Total	Mg	0	0
			2	2		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	1	Total	Zn	0	0
			1	1		

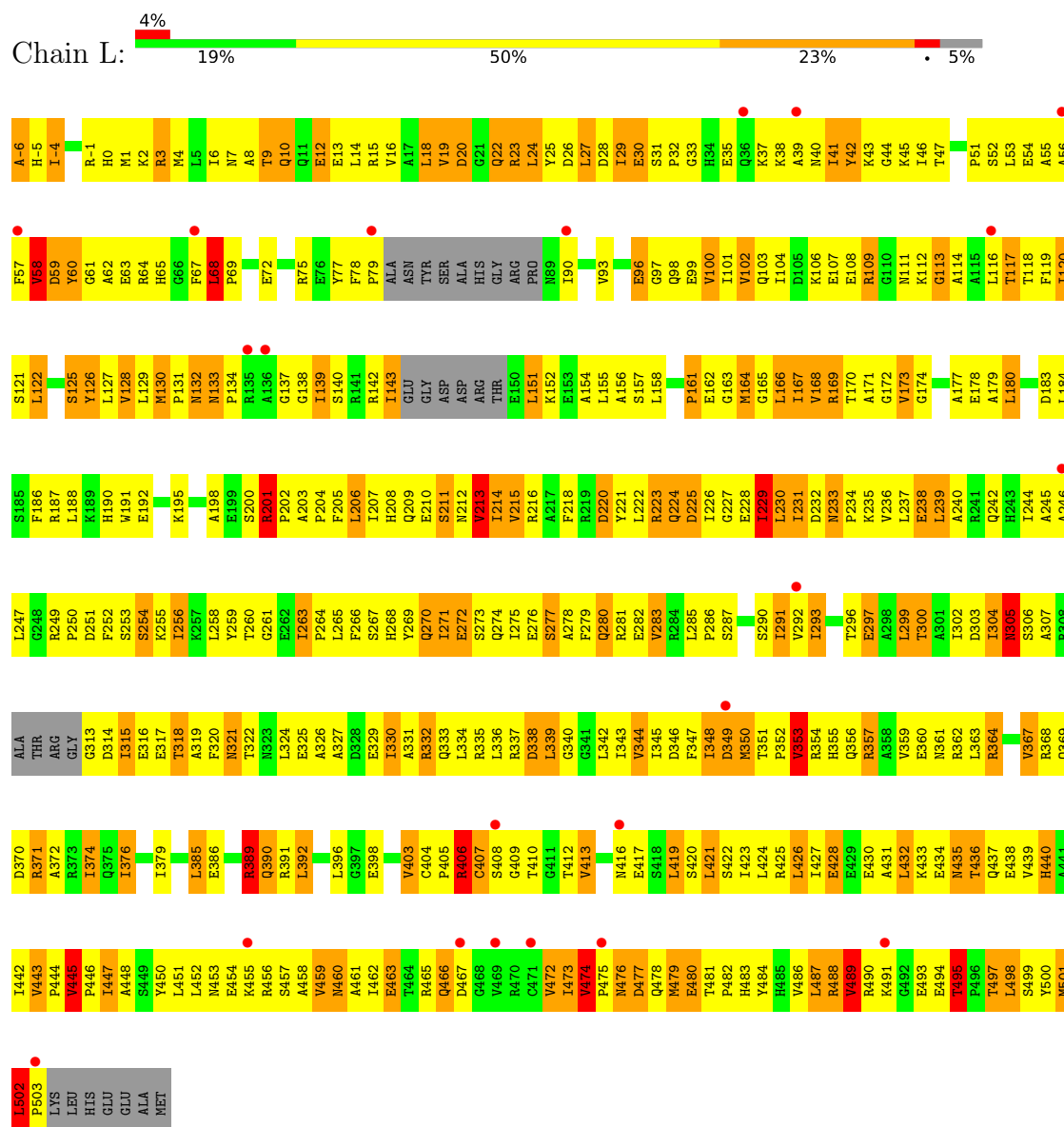
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	5	Total	O	0	0
			5	5		
5	R	1	Total	O	0	0
			1	1		

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: RIBONUCLEASE E



• Molecule 2: SSRNA MOLECULE: 5'-R(*AP*CP*AP*GP*UP*AP*UP*UP*UP*GP)-3'



A1	C2	A3	G4	U5	A6	U7	U8	U9	G10
----	----	----	----	----	----	----	----	----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	196.59Å 196.59Å 140.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 3.60 25.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (25.00-3.60) 99.3 (25.00-3.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.319 , 0.347 0.238 , 0.267	Depositor DCC
R_{free} test set	980 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	122.6	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 109.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3778	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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

5.1 Standard geometry

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

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	L	0.94	8/3610 (0.2%)	1.28	30/4917 (0.6%)
2	R	1.11	2/236 (0.8%)	2.60	27/363 (7.4%)
All	All	0.95	10/3846 (0.3%)	1.41	57/5280 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	21

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	407	CYS	CB-SG	-12.04	1.41	1.81
1	L	407	CYS	C-N	-11.28	1.17	1.33
1	L	472	VAL	CA-CB	-7.32	1.46	1.54
1	L	408	SER	CA-C	-5.98	1.44	1.52
2	R	4	G	C3'-O3'	5.97	1.51	1.42
1	L	344	VAL	CA-CB	-5.83	1.47	1.54
1	L	340	GLY	N-CA	5.19	1.49	1.44
1	L	445	VAL	CA-CB	-5.16	1.51	1.54
2	R	3	A	O5'-C5'	5.10	1.50	1.42
1	L	412	THR	CA-CB	-5.00	1.45	1.53

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	406	ARG	O-C-N	-18.88	102.63	122.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	408	SER	N-CA-C	-13.55	97.68	114.75
2	R	5	U	O4'-C1'-C2'	-12.82	94.78	107.60
2	R	6	A	O4'-C4'-C3'	-12.54	91.47	104.00
2	R	4	G	N9-C1'-C2'	10.91	128.37	112.00
1	L	407	CYS	N-CA-C	-9.92	94.84	109.63
2	R	2	C	O5'-C5'-C4'	-9.73	96.90	111.50
2	R	4	G	C1'-O4'-C4'	-9.67	100.23	109.90
2	R	10	G	C4'-C3'-C2'	-9.58	93.02	102.60
2	R	4	G	P-O3'-C3'	9.26	134.09	120.20
1	L	68	LEU	CA-C-N	8.77	130.80	119.84
1	L	68	LEU	C-N-CA	8.77	130.80	119.84
1	L	406	ARG	CA-C-N	8.24	140.29	122.82
1	L	406	ARG	C-N-CA	8.24	140.29	122.82
2	R	1	A	C1'-O4'-C4'	-8.08	101.62	109.70
1	L	398	GLU	N-CA-C	-7.87	103.40	113.16
1	L	474	VAL	N-CA-C	7.65	115.49	107.76
2	R	4	G	C3'-C2'-C1'	-7.58	93.72	101.30
2	R	4	G	O4'-C1'-C2'	-6.94	100.66	107.60
2	R	2	C	O3'-P-O5'	-6.82	93.76	104.00
2	R	1	A	O4'-C1'-C2'	-6.82	98.98	105.80
1	L	353	VAL	CB-CA-C	-6.80	103.13	112.04
2	R	6	A	O4'-C1'-N9	6.72	118.58	108.50
2	R	1	A	O4'-C1'-N9	6.63	118.14	108.20
1	L	421	LEU	CA-CB-CG	-6.61	93.18	116.30
1	L	416	ASN	N-CA-C	6.58	119.29	111.33
2	R	9	U	P-O3'-C3'	-6.44	110.54	120.20
1	L	220	ASP	N-CA-C	6.26	120.65	112.89
1	L	479	MET	N-CA-C	6.22	119.38	110.24
1	L	19	VAL	N-CA-C	6.21	117.54	108.53
1	L	407	CYS	CA-C-N	-6.11	110.89	121.52
1	L	407	CYS	C-N-CA	-6.11	110.89	121.52
1	L	440	HIS	CB-CA-C	-6.04	102.14	111.74
2	R	7	U	O4'-C1'-C2'	-5.84	101.75	107.60
2	R	4	G	C5'-C4'-C3'	5.81	124.71	116.00
2	R	10	G	O4'-C1'-N9	5.76	117.14	108.50
1	L	305	ASN	N-CA-C	5.72	116.84	108.14
1	L	353	VAL	N-CA-C	5.66	117.07	110.62
2	R	2	C	O4'-C1'-C2'	-5.66	101.94	107.60
1	L	472	VAL	CB-CA-C	-5.65	102.67	111.26
1	L	213	VAL	N-CA-C	5.60	115.80	110.53
2	R	4	G	P-O5'-C5'	5.58	129.28	120.90
1	L	339	LEU	CB-CA-C	-5.56	102.33	110.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	5	U	C4'-C3'-O3'	-5.55	104.68	113.00
2	R	6	A	C3'-C2'-O2'	5.55	119.02	110.70
1	L	229	ILE	CB-CA-C	-5.53	105.65	111.23
2	R	6	A	C1'-O4'-C4'	-5.44	104.46	109.90
1	L	445	VAL	CA-C-N	5.43	124.77	118.85
1	L	445	VAL	C-N-CA	5.43	124.77	118.85
2	R	5	U	O4'-C1'-N1	-5.38	100.43	108.50
1	L	502	LEU	CA-CB-CG	-5.35	97.57	116.30
2	R	5	U	N1-C1'-C2'	5.34	120.02	112.00
1	L	489	VAL	N-CA-C	5.23	115.60	107.28
1	L	271	ILE	CB-CA-C	-5.22	105.28	111.65
1	L	58	VAL	N-CA-C	5.16	116.15	108.46
2	R	1	A	N9-C1'-C2'	5.15	121.73	114.00
2	R	10	G	C1'-O4'-C4'	-5.03	104.87	109.90

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	-6	ALA	Peptide
1	L	109	ARG	Peptide
1	L	113	GLY	Peptide
1	L	130	MET	Peptide
1	L	132	ASN	Peptide
1	L	151	LEU	Peptide
1	L	161	PRO	Peptide
1	L	174	GLY	Peptide
1	L	201	ARG	Peptide
1	L	249	ARG	Peptide
1	L	254	SER	Peptide
1	L	305	ASN	Peptide
1	L	313	GLY	Peptide
1	L	389	ARG	Peptide
1	L	406	ARG	Mainchain
1	L	409	GLY	Peptide
1	L	460	ASN	Peptide
1	L	480	GLU	Peptide
1	L	495	THR	Peptide
1	L	56	ALA	Peptide
1	L	61	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	3557	0	3325	678	0
2	R	212	0	107	67	0
3	L	2	0	0	0	0
4	L	1	0	0	0	0
5	L	5	0	0	4	0
5	R	1	0	0	1	0
All	All	3778	0	3432	719	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 100.

All (719) 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:L:222:LEU:HD23	1:L:226:ILE:CD1	1.28	1.58
1:L:206:LEU:HD12	1:L:207:ILE:N	1.24	1.41
1:L:222:LEU:CD2	1:L:226:ILE:CD1	1.98	1.41
1:L:222:LEU:CD2	1:L:226:ILE:HD12	1.49	1.41
1:L:128:VAL:CG1	1:L:167:ILE:CD1	2.02	1.35
1:L:276:GLU:O	1:L:278:ALA:N	1.61	1.34
2:R:2:C:O2	2:R:2:C:H3'	1.16	1.33
1:L:206:LEU:CD1	1:L:207:ILE:H	1.42	1.31
1:L:128:VAL:HG11	1:L:167:ILE:CD1	1.58	1.30
1:L:458:ALA:O	1:L:461:ALA:HB3	1.26	1.28
1:L:-4:ILE:HD13	1:L:-1:ARG:NH1	1.52	1.25
1:L:259:TYR:CD2	1:L:265:LEU:HG	1.72	1.24
1:L:128:VAL:CG1	1:L:167:ILE:HD13	1.62	1.21
1:L:222:LEU:HD23	1:L:226:ILE:HD13	1.21	1.19
1:L:436:THR:HG23	1:L:488:ARG:HE	1.11	1.15
1:L:102:VAL:HG11	1:L:116:LEU:HD13	1.21	1.15
1:L:143:ILE:HD13	1:L:173:VAL:HG23	1.28	1.14
1:L:128:VAL:CG1	1:L:167:ILE:HD12	1.71	1.13
1:L:222:LEU:HD22	1:L:226:ILE:HD12	1.29	1.13
1:L:10:GLN:HA	1:L:10:GLN:OE1	1.41	1.12
1:L:239:LEU:H	1:L:239:LEU:HD23	1.14	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:2:C:O2	2:R:2:C:C3'	1.97	1.11
1:L:169:ARG:HH11	1:L:169:ARG:CG	1.65	1.10
1:L:184:LEU:O	1:L:188:LEU:HD12	1.51	1.09
1:L:501:MET:HA	1:L:501:MET:HE3	1.11	1.09
1:L:332:ARG:HG2	1:L:332:ARG:HH11	1.15	1.09
1:L:43:LYS:CB	1:L:203:ALA:HB1	1.82	1.08
1:L:473:ILE:HG22	1:L:473:ILE:O	1.47	1.08
1:L:106:LYS:O	1:L:114:ALA:HB1	1.53	1.07
1:L:169:ARG:HG2	1:L:169:ARG:NH1	1.57	1.07
2:R:7:U:H6	2:R:7:U:H5'	1.06	1.06
1:L:169:ARG:NH1	2:R:1:A:OP3	1.88	1.06
1:L:259:TYR:HD2	1:L:265:LEU:HG	0.96	1.06
1:L:239:LEU:HD23	1:L:239:LEU:N	1.65	1.05
1:L:67:PHE:CD1	2:R:10:G:C4	2.47	1.03
1:L:96:GLU:HG2	1:L:97:GLY:H	1.22	1.03
1:L:436:THR:HG23	1:L:488:ARG:NE	1.71	1.03
1:L:348:ILE:CG2	1:L:349:ASP:H	1.71	1.03
1:L:367:VAL:HG21	1:L:374:ILE:HD12	1.03	1.03
2:R:4:G:OP2	2:R:5:U:N3	1.91	1.03
2:R:7:U:H6	2:R:7:U:C5'	1.71	1.02
1:L:140:SER:OG	1:L:170:THR:N	1.91	1.01
1:L:55:ALA:HB2	1:L:69:PRO:HA	1.41	1.01
1:L:130:MET:HB2	1:L:165:GLY:O	1.58	1.01
1:L:293:ILE:HG23	1:L:302:ILE:HG12	1.40	1.01
1:L:137:GLY:O	2:R:2:C:H1'	1.61	1.01
2:R:5:U:H5'	2:R:5:U:C6	1.95	1.01
1:L:501:MET:HA	1:L:501:MET:CE	1.88	1.00
1:L:237:LEU:O	1:L:237:LEU:HD23	1.59	1.00
1:L:367:VAL:CG2	1:L:374:ILE:HD12	1.91	1.00
1:L:143:ILE:HD13	1:L:173:VAL:CG2	1.90	1.00
1:L:235:LYS:O	1:L:238:GLU:HB2	1.60	1.00
1:L:130:MET:O	1:L:164:MET:HB2	1.62	1.00
1:L:7:ASN:HB2	1:L:266:PHE:HE1	1.26	1.00
1:L:169:ARG:HH11	1:L:169:ARG:HG2	0.83	1.00
1:L:259:TYR:HE2	1:L:265:LEU:HA	1.27	0.99
1:L:406:ARG:HE	1:L:481:THR:HG22	1.25	0.98
1:L:233:ASN:ND2	1:L:236:VAL:HG23	1.75	0.98
1:L:57:PHE:HZ	2:R:10:G:HO2'	1.05	0.97
1:L:348:ILE:HG22	1:L:349:ASP:N	1.77	0.97
1:L:143:ILE:CD1	1:L:173:VAL:HG23	1.94	0.96
1:L:481:THR:CG2	1:L:482:PRO:HD3	1.95	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:58:VAL:O	1:L:65:HIS:HB3	1.65	0.96
1:L:129:LEU:HD11	1:L:164:MET:HG3	1.47	0.96
1:L:259:TYR:HD1	1:L:260:THR:N	1.62	0.96
2:R:7:U:H5'	2:R:7:U:C6	1.99	0.96
1:L:18:LEU:O	1:L:25:TYR:CD2	2.20	0.95
1:L:222:LEU:CD2	1:L:226:ILE:HD13	1.78	0.95
2:R:9:U:C5	2:R:10:G:N2	2.35	0.95
1:L:167:ILE:HG12	2:R:2:C:H6	1.31	0.94
1:L:299:LEU:O	1:L:299:LEU:HD12	1.66	0.94
1:L:347:PHE:O	1:L:348:ILE:O	1.85	0.94
2:R:9:U:C6	2:R:10:G:N2	2.36	0.94
1:L:1:MET:HE1	1:L:228:GLU:HG3	1.49	0.93
1:L:230:LEU:N	1:L:230:LEU:HD23	1.84	0.93
1:L:403:VAL:O	1:L:404:CYS:C	2.12	0.93
1:L:180:LEU:N	1:L:180:LEU:HD23	1.83	0.92
2:R:5:U:H3'	2:R:5:U:H6	1.32	0.92
1:L:259:TYR:CE2	1:L:265:LEU:HA	2.04	0.92
1:L:-4:ILE:CD1	1:L:-1:ARG:NH1	2.33	0.92
1:L:348:ILE:CG2	1:L:349:ASP:N	2.30	0.92
1:L:129:LEU:HD12	1:L:130:MET:H	1.32	0.92
2:R:7:U:C5'	2:R:7:U:C6	2.53	0.91
1:L:233:ASN:HD21	1:L:236:VAL:HG23	1.32	0.91
1:L:102:VAL:HG11	1:L:116:LEU:CD1	2.01	0.91
1:L:447:ILE:N	1:L:447:ILE:HD13	1.85	0.90
1:L:130:MET:O	1:L:132:ASN:N	2.04	0.90
1:L:-4:ILE:HD13	1:L:-1:ARG:HH12	1.36	0.89
1:L:131:PRO:HA	1:L:164:MET:CG	2.02	0.89
1:L:67:PHE:HE1	2:R:10:G:H1'	1.38	0.89
1:L:10:GLN:OE1	1:L:10:GLN:CA	2.21	0.89
1:L:203:ALA:N	1:L:204:PRO:CD	2.36	0.88
1:L:128:VAL:HG12	1:L:167:ILE:HD12	1.53	0.88
1:L:265:LEU:HD23	1:L:265:LEU:C	1.95	0.88
1:L:476:ASN:OD1	1:L:477:ASP:N	2.06	0.87
1:L:481:THR:HG23	1:L:482:PRO:HD3	1.54	0.87
1:L:7:ASN:HB2	1:L:266:PHE:CE1	2.10	0.87
1:L:442:ILE:HD13	1:L:474:VAL:HG13	1.56	0.87
1:L:222:LEU:HA	1:L:226:ILE:CD1	2.05	0.87
1:L:-4:ILE:N	1:L:-4:ILE:HD12	1.88	0.87
1:L:332:ARG:HH11	1:L:332:ARG:CG	1.89	0.86
1:L:276:GLU:O	1:L:277:SER:C	2.18	0.86
1:L:334:LEU:HD23	1:L:339:LEU:HD12	1.56	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:129:LEU:HD12	1:L:130:MET:N	1.90	0.86
2:R:2:C:H3'	2:R:2:C:C2	2.11	0.85
1:L:473:ILE:O	1:L:473:ILE:CG2	2.23	0.85
1:L:140:SER:C	1:L:142:ARG:H	1.82	0.85
1:L:205:PHE:CD1	1:L:206:LEU:O	2.29	0.85
1:L:364:ARG:NH2	1:L:364:ARG:HG3	1.90	0.85
1:L:203:ALA:N	1:L:204:PRO:HD3	1.92	0.85
1:L:1:MET:CE	1:L:228:GLU:HG3	2.06	0.85
1:L:291:ILE:O	1:L:291:ILE:HG22	1.77	0.84
1:L:334:LEU:CD2	1:L:339:LEU:HD12	2.07	0.84
1:L:55:ALA:CB	1:L:69:PRO:HA	2.07	0.84
1:L:256:ILE:O	1:L:256:ILE:HG22	1.77	0.84
1:L:406:ARG:HE	1:L:481:THR:CG2	1.91	0.84
1:L:239:LEU:N	1:L:239:LEU:CD2	2.40	0.84
1:L:332:ARG:HG2	1:L:332:ARG:NH1	1.88	0.84
1:L:259:TYR:HE1	1:L:261:GLY:CA	1.91	0.83
2:R:5:U:C6	2:R:5:U:C5'	2.61	0.83
1:L:436:THR:CG2	1:L:488:ARG:HE	1.91	0.83
1:L:259:TYR:HD2	1:L:265:LEU:CG	1.86	0.83
1:L:453:ASN:O	1:L:454:GLU:C	2.21	0.83
1:L:236:VAL:O	1:L:238:GLU:N	2.12	0.83
1:L:299:LEU:O	1:L:299:LEU:CD1	2.25	0.83
1:L:-4:ILE:CD1	1:L:-1:ARG:HH12	1.90	0.83
1:L:44:GLY:O	1:L:100:VAL:N	2.12	0.83
1:L:274:GLN:O	1:L:277:SER:HB3	1.79	0.82
1:L:67:PHE:CE1	2:R:10:G:H1'	2.12	0.82
1:L:483:HIS:O	1:L:484:TYR:HB3	1.79	0.82
2:R:5:U:C6	2:R:5:U:C3'	2.63	0.82
1:L:41:ILE:HG13	1:L:208:HIS:HB3	1.62	0.82
1:L:211:SER:HB2	1:L:215:VAL:HG21	1.60	0.81
1:L:406:ARG:NE	1:L:481:THR:HG22	1.93	0.81
2:R:5:U:C6	2:R:5:U:H3'	2.15	0.81
1:L:42:TYR:CD1	1:L:42:TYR:N	2.45	0.81
1:L:404:CYS:SG	1:L:407:CYS:HB2	2.21	0.80
1:L:42:TYR:N	1:L:42:TYR:HD1	1.79	0.80
1:L:206:LEU:CD1	1:L:207:ILE:N	2.17	0.80
1:L:128:VAL:HG13	1:L:167:ILE:CD1	2.11	0.80
1:L:265:LEU:C	1:L:265:LEU:CD2	2.55	0.80
1:L:498:LEU:HD12	1:L:500:TYR:CZ	2.17	0.80
1:L:237:LEU:O	1:L:237:LEU:CD2	2.30	0.80
1:L:259:TYR:HE1	1:L:261:GLY:HA3	1.45	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:102:VAL:CG1	1:L:116:LEU:HD13	2.08	0.79
1:L:442:ILE:HD13	1:L:474:VAL:CG1	2.12	0.79
1:L:501:MET:HE3	1:L:501:MET:CA	2.03	0.79
1:L:453:ASN:O	1:L:455:LYS:N	2.15	0.79
1:L:222:LEU:HA	1:L:226:ILE:HD11	1.65	0.79
1:L:495:THR:OG1	1:L:497:THR:HB	1.82	0.79
1:L:117:THR:OG1	1:L:119:PHE:HB2	1.82	0.79
1:L:238:GLU:OE2	1:L:238:GLU:HA	1.81	0.79
1:L:29:ILE:CG2	1:L:29:ILE:O	2.30	0.79
1:L:184:LEU:O	1:L:188:LEU:CD1	2.31	0.79
1:L:72:GLU:O	1:L:119:PHE:CD2	2.35	0.79
1:L:458:ALA:O	1:L:461:ALA:CB	2.22	0.79
1:L:364:ARG:HG3	1:L:364:ARG:HH21	1.47	0.79
2:R:4:G:H1'	2:R:5:U:OP2	1.82	0.78
1:L:131:PRO:HA	1:L:164:MET:HG3	1.65	0.78
1:L:346:ASP:OD2	5:L:2003:HOH:O	2.02	0.78
1:L:29:ILE:O	1:L:29:ILE:HG22	1.81	0.78
1:L:259:TYR:CD1	1:L:260:THR:N	2.51	0.78
1:L:-5:HIS:C	1:L:-4:ILE:HD12	2.09	0.78
1:L:7:ASN:ND2	1:L:232:ASP:OD1	2.16	0.78
1:L:137:GLY:O	2:R:2:C:C1'	2.32	0.78
1:L:348:ILE:HG23	1:L:349:ASP:H	1.48	0.78
1:L:169:ARG:NH2	1:L:220:ASP:OD1	2.18	0.77
1:L:305:ASN:HD22	1:L:305:ASN:C	1.93	0.77
1:L:428:GLU:O	1:L:432:LEU:HD22	1.84	0.77
1:L:27:LEU:HG	1:L:28:ASP:N	1.97	0.77
1:L:222:LEU:HD23	1:L:226:ILE:HD12	1.15	0.77
1:L:128:VAL:HG11	1:L:167:ILE:HD13	0.80	0.76
1:L:293:ILE:HG23	1:L:302:ILE:CG1	2.13	0.76
1:L:134:PRO:HD3	1:L:163:GLY:O	1.85	0.76
1:L:367:VAL:CG2	1:L:367:VAL:O	2.33	0.76
1:L:222:LEU:HD23	1:L:226:ILE:HD11	1.62	0.76
1:L:67:PHE:CD1	2:R:10:G:N9	2.54	0.76
1:L:40:ASN:ND2	1:L:209:GLN:HA	2.00	0.76
1:L:476:ASN:OD1	1:L:476:ASN:C	2.28	0.76
2:R:2:C:C3'	2:R:2:C:C2	2.69	0.75
1:L:367:VAL:HG21	1:L:374:ILE:CD1	2.00	0.75
1:L:55:ALA:HB1	1:L:68:LEU:O	1.87	0.75
1:L:201:ARG:HG3	1:L:202:PRO:O	1.86	0.75
1:L:237:LEU:HA	1:L:240:ALA:CB	2.17	0.74
1:L:304:ILE:HD11	1:L:330:ILE:HD11	1.67	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:450:TYR:CE1	1:L:454:GLU:HG2	2.22	0.74
1:L:233:ASN:ND2	1:L:236:VAL:CG2	2.49	0.74
1:L:372:ALA:HB2	1:L:392:LEU:HG	1.68	0.74
1:L:22:GLN:HG2	1:L:269:TYR:O	1.86	0.74
1:L:128:VAL:CG1	1:L:128:VAL:O	2.36	0.74
1:L:276:GLU:C	1:L:278:ALA:N	2.45	0.73
1:L:244:ILE:O	1:L:245:ALA:C	2.31	0.73
1:L:41:ILE:HG23	1:L:103:GLN:HB2	1.69	0.73
1:L:103:GLN:HG3	1:L:104:ILE:H	1.54	0.73
1:L:212:ASN:OD1	1:L:214:ILE:N	2.21	0.73
1:L:1:MET:HE2	1:L:227:GLY:HA3	1.70	0.72
1:L:291:ILE:HD13	1:L:330:ILE:HG13	1.71	0.72
2:R:9:U:OP1	5:R:2001:HOH:O	2.05	0.72
1:L:131:PRO:HA	1:L:164:MET:CB	2.19	0.72
1:L:40:ASN:C	1:L:41:ILE:HG12	2.14	0.72
1:L:38:LYS:O	1:L:39:ALA:HB3	1.90	0.72
1:L:346:ASP:OD2	5:L:2004:HOH:O	2.06	0.72
1:L:370:ASP:OD1	1:L:389:ARG:NH2	2.22	0.71
1:L:481:THR:HG23	1:L:482:PRO:CD	2.20	0.71
2:R:4:G:H4'	2:R:5:U:C5'	2.20	0.71
1:L:423:ILE:HD11	1:L:484:TYR:CD2	2.25	0.71
1:L:481:THR:HG22	1:L:482:PRO:HD3	1.71	0.71
1:L:31:SER:O	1:L:32:PRO:O	2.09	0.71
1:L:96:GLU:HG2	1:L:97:GLY:N	1.87	0.71
1:L:237:LEU:O	1:L:240:ALA:HB3	1.90	0.71
1:L:203:ALA:O	1:L:205:PHE:N	2.22	0.71
1:L:259:TYR:HE1	1:L:261:GLY:N	1.88	0.71
1:L:131:PRO:C	1:L:164:MET:HB3	2.16	0.71
1:L:122:LEU:O	1:L:128:VAL:HA	1.90	0.70
1:L:140:SER:C	1:L:142:ARG:N	2.45	0.70
1:L:465:ARG:O	1:L:467:ASP:N	2.23	0.70
2:R:5:U:H2'	2:R:6:A:O5'	1.91	0.70
1:L:130:MET:CB	1:L:165:GLY:O	2.37	0.70
1:L:41:ILE:O	1:L:207:ILE:HB	1.91	0.70
1:L:297:GLU:HG3	1:L:297:GLU:O	1.91	0.70
1:L:2:LYS:HA	1:L:20:ASP:HA	1.74	0.70
1:L:67:PHE:CD2	1:L:69:PRO:HD3	2.27	0.70
1:L:132:ASN:CG	1:L:132:ASN:O	2.35	0.70
1:L:443:VAL:HG23	1:L:447:ILE:HB	1.74	0.70
1:L:447:ILE:HD13	1:L:447:ILE:H	1.56	0.69
1:L:75:ARG:O	1:L:78:PHE:CB	2.40	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:317:GLU:OE1	1:L:321:ASN:HB2	1.92	0.69
1:L:445:VAL:HG12	1:L:446:PRO:CD	2.22	0.69
1:L:348:ILE:HG22	1:L:349:ASP:H	1.37	0.69
1:L:72:GLU:O	1:L:119:PHE:HD2	1.74	0.69
1:L:138:GLY:HA3	2:R:2:C:O2'	1.92	0.69
1:L:177:ALA:O	1:L:178:GLU:C	2.34	0.69
1:L:350:MET:SD	1:L:355:HIS:HB3	2.32	0.69
1:L:372:ALA:HB1	1:L:390:GLN:HG2	1.75	0.69
1:L:58:VAL:O	1:L:65:HIS:CB	2.41	0.69
1:L:167:ILE:HG12	2:R:2:C:C6	2.23	0.68
1:L:266:PHE:CD2	1:L:271:ILE:HD11	2.28	0.68
2:R:5:U:C2'	2:R:6:A:O5'	2.41	0.68
1:L:460:ASN:O	1:L:462:ILE:N	2.27	0.68
1:L:128:VAL:HG12	1:L:167:ILE:CD1	2.11	0.68
2:R:9:U:H6	2:R:10:G:H21	1.39	0.68
1:L:259:TYR:CE1	1:L:261:GLY:N	2.61	0.68
1:L:369:GLN:O	1:L:370:ASP:C	2.34	0.68
1:L:62:ALA:O	1:L:63:GLU:C	2.36	0.68
1:L:476:ASN:OD1	1:L:478:GLN:N	2.24	0.68
1:L:390:GLN:NE2	2:R:6:A:H5'	2.09	0.68
1:L:447:ILE:N	1:L:447:ILE:CD1	2.57	0.68
1:L:-6:ALA:O	1:L:-4:ILE:CD1	2.42	0.68
1:L:203:ALA:O	1:L:205:PHE:CD2	2.46	0.68
1:L:347:PHE:C	1:L:348:ILE:O	2.35	0.68
1:L:448:ALA:HB3	1:L:475:PRO:HB3	1.75	0.67
1:L:2:LYS:HG2	1:L:20:ASP:HB2	1.75	0.67
1:L:125:SER:O	1:L:169:ARG:HD3	1.95	0.67
1:L:484:TYR:CD1	1:L:484:TYR:C	2.73	0.67
1:L:25:TYR:O	1:L:26:ASP:HB2	1.94	0.67
1:L:445:VAL:HG12	1:L:446:PRO:N	2.08	0.67
1:L:481:THR:N	1:L:482:PRO:CD	2.58	0.67
1:L:128:VAL:HG13	1:L:167:ILE:HD12	1.69	0.67
1:L:237:LEU:C	1:L:240:ALA:HB3	2.19	0.67
1:L:67:PHE:HD1	2:R:10:G:C8	2.13	0.67
1:L:103:GLN:HG3	1:L:104:ILE:N	2.10	0.66
1:L:205:PHE:CE1	1:L:206:LEU:O	2.48	0.66
1:L:238:GLU:OE2	1:L:238:GLU:CA	2.43	0.66
1:L:303:ASP:OD2	5:L:2001:HOH:O	2.12	0.66
1:L:486:VAL:HG12	1:L:486:VAL:O	1.94	0.66
1:L:130:MET:C	1:L:164:MET:HB2	2.20	0.66
1:L:417:GLU:N	1:L:417:GLU:OE2	2.26	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:126:TYR:HD1	1:L:172:GLY:HA2	1.61	0.66
1:L:151:LEU:O	1:L:155:LEU:N	2.26	0.65
1:L:212:ASN:OD1	1:L:213:VAL:N	2.28	0.65
1:L:466:GLN:HA	1:L:466:GLN:NE2	2.11	0.65
1:L:45:LYS:HA	1:L:98:GLN:O	1.95	0.65
1:L:367:VAL:O	1:L:367:VAL:HG22	1.96	0.65
1:L:120:ILE:N	1:L:120:ILE:HD12	2.11	0.65
1:L:202:PRO:C	1:L:204:PRO:HD2	2.22	0.65
1:L:403:VAL:O	1:L:405:PRO:N	2.29	0.65
1:L:236:VAL:C	1:L:238:GLU:N	2.54	0.65
1:L:259:TYR:CD1	1:L:259:TYR:C	2.73	0.65
1:L:134:PRO:HA	1:L:165:GLY:N	2.10	0.65
2:R:2:C:O2'	2:R:3:A:P	2.55	0.65
2:R:9:U:H5	2:R:10:G:H22	1.41	0.65
1:L:137:GLY:O	2:R:2:C:C2'	2.45	0.65
1:L:494:GLU:HG2	1:L:494:GLU:O	1.96	0.65
1:L:502:LEU:O	1:L:503:PRO:C	2.40	0.65
1:L:212:ASN:OD1	1:L:212:ASN:C	2.39	0.64
1:L:404:CYS:SG	1:L:404:CYS:O	2.55	0.64
1:L:67:PHE:CE1	2:R:10:G:C4	2.85	0.64
1:L:223:ARG:HB2	1:L:225:ASP:OD2	1.98	0.64
1:L:12:GLU:O	1:L:13:GLU:HB2	1.97	0.64
1:L:55:ALA:HB1	1:L:68:LEU:C	2.23	0.64
1:L:443:VAL:HG21	1:L:447:ILE:HG22	1.80	0.64
1:L:180:LEU:N	1:L:180:LEU:CD2	2.57	0.64
1:L:286:PRO:HB2	1:L:325:GLU:OE1	1.98	0.63
1:L:291:ILE:O	1:L:291:ILE:CG2	2.46	0.63
1:L:319:ALA:HB1	1:L:348:ILE:HG21	1.80	0.63
1:L:436:THR:CG2	1:L:488:ARG:NE	2.55	0.63
1:L:203:ALA:H	1:L:204:PRO:HD3	1.63	0.63
1:L:259:TYR:CE2	1:L:265:LEU:HG	2.30	0.63
1:L:335:ARG:HG3	1:L:335:ARG:HH11	1.63	0.63
2:R:4:G:H4'	2:R:5:U:H5'	1.79	0.63
1:L:259:TYR:CD2	1:L:265:LEU:CG	2.65	0.63
2:R:5:U:H5'	2:R:5:U:C5	2.34	0.63
1:L:259:TYR:HD1	1:L:260:THR:H	1.45	0.62
1:L:41:ILE:C	1:L:42:TYR:CD1	2.76	0.62
1:L:224:GLN:HA	1:L:224:GLN:NE2	2.09	0.62
1:L:260:THR:O	1:L:261:GLY:C	2.42	0.62
1:L:-4:ILE:CD1	1:L:-4:ILE:N	2.55	0.62
1:L:108:GLU:HA	1:L:113:GLY:O	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:234:PRO:HG3	1:L:258:LEU:HD11	1.82	0.62
1:L:270:GLN:OE1	1:L:270:GLN:HA	2.00	0.62
1:L:436:THR:CG2	1:L:488:ARG:HG3	2.30	0.62
1:L:353:VAL:HA	1:L:356:GLN:NE2	2.15	0.61
2:R:4:G:OP2	2:R:5:U:C2	2.53	0.61
1:L:62:ALA:O	1:L:63:GLU:O	2.18	0.61
1:L:67:PHE:CE1	2:R:10:G:C1'	2.83	0.61
1:L:170:THR:CG2	1:L:170:THR:O	2.48	0.61
1:L:60:TYR:H	1:L:60:TYR:HD2	1.49	0.61
1:L:-1:ARG:HG2	1:L:0:HIS:CE1	2.36	0.60
1:L:452:LEU:O	1:L:456:ARG:HB2	2.00	0.60
1:L:477:ASP:N	1:L:477:ASP:OD2	2.34	0.60
1:L:30:GLU:OE2	1:L:213:VAL:N	2.35	0.60
1:L:259:TYR:CE1	1:L:261:GLY:CA	2.81	0.60
1:L:51:PRO:C	1:L:53:LEU:H	2.09	0.60
1:L:187:ARG:O	1:L:188:LEU:C	2.45	0.60
1:L:188:LEU:HA	1:L:191:TRP:HB3	1.83	0.60
1:L:236:VAL:O	1:L:237:LEU:C	2.44	0.60
1:L:304:ILE:HD11	1:L:330:ILE:CD1	2.31	0.60
1:L:306:SER:OG	1:L:307:ALA:N	2.34	0.60
2:R:2:C:O2	2:R:2:C:C2'	2.49	0.60
1:L:101:ILE:O	1:L:120:ILE:HD11	2.02	0.60
1:L:103:GLN:CG	1:L:104:ILE:N	2.65	0.60
1:L:127:LEU:HD21	1:L:168:VAL:HG13	1.83	0.60
2:R:6:A:H2'	2:R:7:U:H5''	1.82	0.60
1:L:166:LEU:C	1:L:166:LEU:HD23	2.27	0.60
1:L:237:LEU:CD2	1:L:237:LEU:C	2.75	0.60
1:L:317:GLU:O	1:L:318:THR:C	2.45	0.60
1:L:457:SER:O	1:L:461:ALA:HB2	2.00	0.60
1:L:259:TYR:HD1	1:L:259:TYR:C	2.08	0.59
1:L:53:LEU:O	1:L:54:GLU:CB	2.50	0.59
1:L:131:PRO:CA	1:L:164:MET:CB	2.80	0.59
2:R:4:G:P	2:R:5:U:H3	2.23	0.59
1:L:137:GLY:HA2	1:L:166:LEU:O	2.03	0.59
1:L:237:LEU:HA	1:L:240:ALA:HB2	1.83	0.59
1:L:132:ASN:N	1:L:164:MET:HB3	2.18	0.59
1:L:239:LEU:O	1:L:240:ALA:C	2.44	0.59
1:L:431:ALA:O	1:L:466:GLN:HG3	2.02	0.59
1:L:466:GLN:O	1:L:467:ASP:C	2.45	0.59
1:L:170:THR:O	1:L:170:THR:HG22	2.01	0.59
1:L:60:TYR:HE1	1:L:104:ILE:HD11	1.67	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:180:LEU:HD23	1:L:180:LEU:H	1.63	0.58
1:L:454:GLU:N	1:L:454:GLU:OE1	2.33	0.58
1:L:77:TYR:O	1:L:79:PRO:HD3	2.04	0.58
1:L:154:ALA:HB1	1:L:177:ALA:HB2	1.85	0.58
1:L:246:ALA:O	1:L:247:LEU:C	2.45	0.58
1:L:291:ILE:CD1	1:L:330:ILE:HG13	2.32	0.58
1:L:43:LYS:CB	1:L:203:ALA:CB	2.72	0.58
1:L:44:GLY:N	1:L:100:VAL:O	2.35	0.58
1:L:448:ALA:CB	1:L:475:PRO:HB3	2.32	0.58
2:R:5:U:C6	2:R:5:U:C4'	2.85	0.58
1:L:169:ARG:C	1:L:171:ALA:H	2.10	0.58
1:L:122:LEU:O	1:L:129:LEU:N	2.34	0.58
1:L:133:ASN:O	1:L:133:ASN:ND2	2.37	0.58
1:L:279:PHE:CZ	1:L:396:LEU:HD21	2.39	0.58
1:L:67:PHE:CD1	2:R:10:G:C5	2.91	0.57
1:L:109:ARG:O	1:L:111:ASN:N	2.37	0.57
1:L:140:SER:O	1:L:142:ARG:N	2.37	0.57
1:L:8:ALA:CB	1:L:236:VAL:HG21	2.34	0.57
1:L:55:ALA:CB	1:L:69:PRO:CA	2.80	0.57
1:L:128:VAL:HG13	1:L:128:VAL:O	2.05	0.57
1:L:259:TYR:CE1	1:L:261:GLY:HA3	2.32	0.57
1:L:131:PRO:HB2	1:L:191:TRP:CE2	2.39	0.57
1:L:67:PHE:HE1	2:R:10:G:C1'	2.14	0.57
1:L:-4:ILE:HD13	1:L:-1:ARG:CZ	2.28	0.57
1:L:166:LEU:HD23	1:L:166:LEU:O	2.03	0.57
1:L:41:ILE:C	1:L:42:TYR:HD1	2.11	0.57
1:L:58:VAL:C	1:L:65:HIS:HB3	2.28	0.56
1:L:370:ASP:CG	1:L:389:ARG:HH21	2.11	0.56
1:L:102:VAL:HG13	1:L:116:LEU:HB3	1.87	0.56
1:L:1:MET:CE	1:L:227:GLY:HA3	2.36	0.56
1:L:6:ILE:HB	1:L:231:ILE:HG13	1.86	0.56
1:L:18:LEU:O	1:L:25:TYR:CE2	2.57	0.56
1:L:38:LYS:O	1:L:39:ALA:CB	2.53	0.56
1:L:40:ASN:HB3	1:L:42:TYR:HE1	1.71	0.56
2:R:6:A:C6	2:R:7:U:N3	2.74	0.56
1:L:360:GLU:OE2	1:L:379:ILE:N	2.36	0.56
1:L:498:LEU:HB2	1:L:501:MET:HB2	1.88	0.56
1:L:391:ARG:NH2	2:R:8:U:OP1	2.38	0.56
1:L:498:LEU:HD12	1:L:500:TYR:OH	2.06	0.56
1:L:3:ARG:N	1:L:19:VAL:O	2.36	0.56
1:L:40:ASN:HB3	1:L:42:TYR:CE1	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:188:LEU:O	1:L:191:TRP:N	2.38	0.56
1:L:303:ASP:OD2	5:L:2004:HOH:O	2.17	0.56
1:L:265:LEU:HD23	1:L:265:LEU:O	2.06	0.56
1:L:314:ASP:OD1	1:L:315:ILE:N	2.39	0.56
1:L:445:VAL:CG1	1:L:446:PRO:N	2.67	0.56
1:L:132:ASN:N	1:L:164:MET:CB	2.69	0.56
1:L:357:ARG:NH1	1:L:360:GLU:OE2	2.39	0.56
1:L:445:VAL:N	1:L:446:PRO:CD	2.69	0.56
1:L:498:LEU:O	1:L:499:SER:C	2.48	0.56
1:L:120:ILE:N	1:L:120:ILE:CD1	2.68	0.56
1:L:1:MET:HE2	1:L:227:GLY:CA	2.35	0.55
1:L:167:ILE:HG22	1:L:168:VAL:H	1.70	0.55
1:L:58:VAL:HG21	1:L:116:LEU:HD12	1.87	0.55
1:L:127:LEU:CD2	1:L:168:VAL:HG13	2.36	0.55
1:L:140:SER:HB2	1:L:143:ILE:HG13	1.89	0.55
1:L:299:LEU:CD1	1:L:299:LEU:C	2.78	0.55
1:L:30:GLU:HB2	1:L:213:VAL:HB	1.88	0.55
1:L:161:PRO:HB2	1:L:164:MET:HE1	1.88	0.55
1:L:59:ASP:OD1	1:L:65:HIS:CD2	2.60	0.55
1:L:276:GLU:O	1:L:279:PHE:N	2.38	0.55
1:L:202:PRO:C	1:L:204:PRO:CD	2.79	0.55
1:L:19:VAL:HG13	1:L:23:ARG:O	2.07	0.55
1:L:320:PHE:HB2	1:L:355:HIS:CD2	2.41	0.55
1:L:27:LEU:CG	1:L:28:ASP:N	2.70	0.55
1:L:67:PHE:CD1	2:R:10:G:C8	2.95	0.55
1:L:107:GLU:O	1:L:108:GLU:C	2.50	0.55
1:L:391:ARG:HH21	2:R:8:U:P	2.30	0.55
1:L:450:TYR:CD1	1:L:454:GLU:HG2	2.42	0.55
1:L:252:PHE:HA	1:L:255:LYS:HB2	1.87	0.55
1:L:458:ALA:C	1:L:461:ALA:HB3	2.20	0.54
1:L:465:ARG:C	1:L:467:ASP:H	2.13	0.54
1:L:22:GLN:O	1:L:274:GLN:NE2	2.38	0.54
1:L:265:LEU:HD21	1:L:269:TYR:HD1	1.72	0.54
1:L:351:THR:N	1:L:352:PRO:HD2	2.23	0.54
1:L:140:SER:OG	1:L:170:THR:CA	2.54	0.54
1:L:347:PHE:HE2	1:L:385:LEU:HD22	1.72	0.54
1:L:465:ARG:C	1:L:467:ASP:N	2.64	0.54
1:L:413:VAL:HG11	1:L:481:THR:HG21	1.89	0.54
1:L:190:HIS:O	1:L:192:GLU:N	2.40	0.54
1:L:263:ILE:HG23	1:L:264:PRO:HD2	1.89	0.54
1:L:119:PHE:HA	1:L:132:ASN:ND2	2.22	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:490:ARG:O	1:L:491:LYS:O	2.26	0.54
1:L:96:GLU:CG	1:L:97:GLY:N	2.66	0.54
1:L:251:ASP:O	1:L:252:PHE:CD1	2.61	0.54
2:R:2:C:O2'	2:R:3:A:OP1	2.26	0.54
1:L:127:LEU:HD12	1:L:183:ASP:HB3	1.89	0.53
1:L:187:ARG:O	1:L:190:HIS:N	2.42	0.53
1:L:213:VAL:HG13	1:L:214:ILE:N	2.23	0.53
1:L:490:ARG:O	1:L:491:LYS:C	2.50	0.53
1:L:1:MET:HE2	1:L:228:GLU:N	2.23	0.53
1:L:130:MET:C	1:L:132:ASN:N	2.64	0.53
1:L:237:LEU:HA	1:L:240:ALA:HB3	1.90	0.53
1:L:112:LYS:CB	2:R:10:G:C5	2.91	0.53
1:L:198:ALA:C	1:L:200:SER:N	2.64	0.53
1:L:229:ILE:HB	1:L:256:ILE:HG12	1.91	0.53
1:L:33:GLY:O	1:L:35:GLU:N	2.37	0.53
1:L:128:VAL:HG12	1:L:128:VAL:O	2.08	0.53
1:L:213:VAL:CG1	1:L:214:ILE:N	2.70	0.53
1:L:30:GLU:CB	1:L:213:VAL:HB	2.38	0.53
1:L:155:LEU:O	1:L:158:LEU:CB	2.57	0.53
1:L:203:ALA:C	1:L:205:PHE:CD2	2.87	0.53
1:L:368:ARG:CG	1:L:368:ARG:NH1	2.72	0.53
1:L:460:ASN:O	1:L:461:ALA:C	2.52	0.53
1:L:177:ALA:O	1:L:179:ALA:N	2.41	0.53
1:L:337:ARG:O	1:L:338:ASP:C	2.49	0.53
1:L:479:MET:SD	1:L:484:TYR:HA	2.50	0.52
1:L:434:GLU:O	1:L:435:ASN:CB	2.57	0.52
1:L:8:ALA:HB3	1:L:233:ASN:HD22	1.74	0.52
1:L:490:ARG:O	1:L:493:GLU:HG2	2.09	0.52
1:L:167:ILE:HD12	1:L:167:ILE:H	1.74	0.52
1:L:329:GLU:OE1	1:L:332:ARG:NH1	2.42	0.52
1:L:233:ASN:HD22	1:L:236:VAL:CG2	2.21	0.52
1:L:271:ILE:O	1:L:271:ILE:HG13	2.10	0.52
1:L:367:VAL:O	1:L:367:VAL:HG23	2.09	0.52
1:L:55:ALA:HB2	1:L:69:PRO:CA	2.28	0.52
1:L:140:SER:OG	1:L:169:ARG:C	2.52	0.52
1:L:359:VAL:O	1:L:362:ARG:HB3	2.09	0.52
1:L:362:ARG:HD2	1:L:362:ARG:O	2.10	0.52
1:L:498:LEU:HD12	1:L:500:TYR:CE2	2.44	0.52
1:L:4:MET:CE	1:L:18:LEU:HD21	2.40	0.52
1:L:8:ALA:HB1	1:L:236:VAL:HG21	1.92	0.52
1:L:203:ALA:C	1:L:205:PHE:HD2	2.18	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:237:LEU:CD1	1:L:258:LEU:HB2	2.39	0.52
2:R:4:G:H4'	2:R:5:U:H5''	1.91	0.52
1:L:40:ASN:CB	1:L:42:TYR:HE1	2.22	0.52
1:L:222:LEU:HA	1:L:226:ILE:HD12	1.79	0.52
1:L:131:PRO:C	1:L:164:MET:CB	2.83	0.52
1:L:214:ILE:HG22	1:L:215:VAL:N	2.24	0.52
1:L:291:ILE:HG12	1:L:304:ILE:HG13	1.91	0.52
1:L:356:GLN:O	1:L:360:GLU:HG3	2.10	0.52
1:L:58:VAL:CG2	1:L:116:LEU:HD12	2.40	0.51
1:L:242:GLN:O	1:L:245:ALA:HB3	2.10	0.51
1:L:333:GLN:O	1:L:334:LEU:C	2.50	0.51
1:L:134:PRO:HA	1:L:164:MET:C	2.35	0.51
1:L:237:LEU:CA	1:L:240:ALA:CB	2.88	0.51
1:L:237:LEU:HD12	1:L:258:LEU:HB2	1.92	0.51
1:L:299:LEU:O	1:L:299:LEU:HD13	2.10	0.51
1:L:426:LEU:HD12	1:L:426:LEU:C	2.35	0.51
1:L:126:TYR:CD2	1:L:126:TYR:N	2.79	0.51
1:L:436:THR:HG22	1:L:488:ARG:HG3	1.92	0.51
1:L:272:GLU:O	1:L:275:ILE:N	2.44	0.51
1:L:285:LEU:O	1:L:286:PRO:C	2.53	0.51
1:L:113:GLY:N	2:R:10:G:N7	2.41	0.51
1:L:272:GLU:O	1:L:273:SER:C	2.54	0.51
1:L:424:LEU:HB2	1:L:451:LEU:CD2	2.40	0.51
2:R:8:U:H5''	2:R:9:U:OP2	2.10	0.51
1:L:279:PHE:CE2	1:L:396:LEU:HD21	2.46	0.51
1:L:134:PRO:HG3	1:L:162:GLU:O	2.11	0.51
1:L:237:LEU:CA	1:L:240:ALA:HB3	2.41	0.51
1:L:-6:ALA:O	1:L:-4:ILE:HD11	2.11	0.50
1:L:151:LEU:O	1:L:152:LYS:C	2.53	0.50
1:L:481:THR:CG2	1:L:482:PRO:CD	2.78	0.50
1:L:8:ALA:CB	1:L:233:ASN:HD22	2.25	0.50
1:L:67:PHE:HB2	2:R:10:G:C5	2.47	0.50
1:L:16:VAL:HG12	1:L:16:VAL:O	2.11	0.50
1:L:119:PHE:CD1	1:L:133:ASN:OD1	2.64	0.50
1:L:198:ALA:C	1:L:200:SER:H	2.19	0.50
1:L:117:THR:C	1:L:119:PHE:H	2.18	0.50
1:L:223:ARG:H	1:L:226:ILE:CD1	2.25	0.50
2:R:5:U:C5	2:R:6:A:C2	2.99	0.50
1:L:369:GLN:O	1:L:370:ASP:O	2.30	0.50
1:L:456:ARG:HG2	1:L:460:ASN:ND2	2.26	0.50
1:L:481:THR:O	1:L:481:THR:OG1	2.25	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1:MET:HE2	1:L:228:GLU:HG3	1.93	0.50
1:L:44:GLY:O	1:L:99:GLU:HA	2.11	0.50
1:L:315:ILE:O	1:L:316:GLU:C	2.55	0.50
1:L:137:GLY:CA	1:L:166:LEU:O	2.60	0.50
1:L:272:GLU:O	1:L:275:ILE:HB	2.12	0.50
1:L:132:ASN:H	1:L:164:MET:HB2	1.77	0.49
1:L:167:ILE:HD12	1:L:167:ILE:N	2.27	0.49
1:L:265:LEU:O	1:L:268:HIS:N	2.38	0.49
1:L:423:ILE:HD11	1:L:484:TYR:CG	2.47	0.49
1:L:305:ASN:C	1:L:305:ASN:ND2	2.64	0.49
1:L:422:SER:O	1:L:423:ILE:C	2.55	0.49
1:L:327:ALA:CB	1:L:362:ARG:HG3	2.43	0.49
1:L:67:PHE:CE1	2:R:10:G:N9	2.80	0.49
1:L:222:LEU:HD21	1:L:226:ILE:HD13	1.81	0.49
1:L:-6:ALA:O	1:L:-4:ILE:HD12	2.12	0.49
1:L:462:ILE:HG22	1:L:463:GLU:N	2.28	0.49
1:L:20:ASP:OD1	1:L:20:ASP:O	2.30	0.49
1:L:58:VAL:O	1:L:65:HIS:CA	2.61	0.49
2:R:5:U:H5'	2:R:5:U:N1	2.25	0.49
1:L:143:ILE:CD1	1:L:173:VAL:CG2	2.71	0.49
1:L:119:PHE:CE1	1:L:133:ASN:OD1	2.67	0.48
1:L:426:LEU:HD12	1:L:426:LEU:O	2.14	0.48
1:L:260:THR:O	1:L:261:GLY:O	2.30	0.48
1:L:443:VAL:HG21	1:L:447:ILE:CG2	2.42	0.48
1:L:192:GLU:O	1:L:195:LYS:N	2.41	0.48
1:L:139:ILE:HG23	1:L:168:VAL:HG23	1.95	0.48
1:L:154:ALA:O	1:L:157:SER:OG	2.25	0.48
2:R:4:G:H1'	2:R:5:U:P	2.52	0.48
1:L:1:MET:HE2	1:L:227:GLY:C	2.38	0.48
1:L:169:ARG:C	1:L:171:ALA:N	2.71	0.48
1:L:190:HIS:O	1:L:191:TRP:C	2.55	0.48
1:L:128:VAL:HG12	1:L:167:ILE:H	1.79	0.48
1:L:376:ILE:O	1:L:376:ILE:HG22	2.13	0.48
1:L:205:PHE:CD1	1:L:205:PHE:C	2.92	0.48
1:L:320:PHE:HB2	1:L:355:HIS:HD2	1.79	0.47
1:L:252:PHE:C	1:L:255:LYS:H	2.22	0.47
1:L:363:LEU:HD12	1:L:363:LEU:HA	1.54	0.47
1:L:474:VAL:O	1:L:474:VAL:HG22	2.12	0.47
1:L:134:PRO:HA	1:L:165:GLY:CA	2.44	0.47
1:L:445:VAL:N	1:L:446:PRO:HD3	2.30	0.47
1:L:493:GLU:O	1:L:493:GLU:HG3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:72:GLU:O	1:L:119:PHE:CE2	2.68	0.47
1:L:46:ILE:HD12	1:L:98:GLN:H	1.79	0.47
1:L:225:ASP:OD2	1:L:225:ASP:N	2.47	0.47
1:L:103:GLN:O	1:L:116:LEU:HA	2.15	0.47
1:L:237:LEU:HD23	1:L:237:LEU:C	2.23	0.47
1:L:361:ASN:O	1:L:362:ARG:C	2.58	0.47
1:L:432:LEU:O	1:L:434:GLU:N	2.47	0.47
2:R:7:U:C6	2:R:7:U:H5'	2.44	0.47
1:L:453:ASN:C	1:L:455:LYS:N	2.73	0.46
1:L:432:LEU:CD1	1:L:466:GLN:CD	2.88	0.46
1:L:443:VAL:CG2	1:L:447:ILE:HB	2.42	0.46
1:L:120:ILE:O	1:L:131:PRO:HD2	2.16	0.46
1:L:231:ILE:HG22	1:L:233:ASN:H	1.80	0.46
1:L:363:LEU:O	1:L:364:ARG:C	2.59	0.46
1:L:-4:ILE:HD11	1:L:-1:ARG:HH12	1.75	0.46
1:L:132:ASN:O	1:L:133:ASN:HB3	2.16	0.46
1:L:364:ARG:HH21	1:L:364:ARG:CG	2.15	0.46
1:L:438:GLU:C	1:L:489:VAL:HG23	2.40	0.46
1:L:250:PRO:C	1:L:252:PHE:H	2.24	0.46
1:L:319:ALA:CB	1:L:348:ILE:HG21	2.45	0.46
1:L:203:ALA:HA	1:L:205:PHE:CE2	2.51	0.46
1:L:215:VAL:O	1:L:216:ARG:C	2.58	0.46
1:L:423:ILE:HD11	1:L:484:TYR:CE2	2.50	0.46
1:L:456:ARG:O	1:L:459:VAL:HG23	2.16	0.46
1:L:154:ALA:CB	1:L:177:ALA:HB2	2.45	0.46
1:L:305:ASN:HA	1:L:348:ILE:HD11	1.96	0.46
1:L:440:HIS:ND1	1:L:502:LEU:HD13	2.30	0.46
1:L:15:ARG:HG2	1:L:29:ILE:CG1	2.45	0.46
1:L:19:VAL:HG13	1:L:23:ARG:C	2.41	0.46
1:L:58:VAL:HB	1:L:116:LEU:HD11	1.96	0.46
1:L:345:ILE:HG21	1:L:347:PHE:CZ	2.51	0.46
1:L:198:ALA:O	1:L:200:SER:N	2.49	0.46
1:L:222:LEU:C	1:L:223:ARG:HG2	2.41	0.46
1:L:417:GLU:O	1:L:420:SER:N	2.49	0.45
1:L:126:TYR:CD1	1:L:172:GLY:HA2	2.45	0.45
1:L:251:ASP:O	1:L:251:ASP:CG	2.55	0.45
1:L:428:GLU:O	1:L:428:GLU:HG3	2.15	0.45
1:L:460:ASN:C	1:L:462:ILE:N	2.74	0.45
1:L:236:VAL:C	1:L:238:GLU:H	2.24	0.45
1:L:302:ILE:HD13	1:L:330:ILE:HG12	1.97	0.45
1:L:324:LEU:O	1:L:327:ALA:HB3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:336:LEU:HD23	1:L:336:LEU:HA	1.59	0.45
1:L:120:ILE:HG22	1:L:122:LEU:HD12	1.98	0.45
1:L:451:LEU:HD13	1:L:473:ILE:HD13	1.98	0.45
1:L:462:ILE:O	1:L:463:GLU:C	2.60	0.45
1:L:75:ARG:O	1:L:78:PHE:N	2.48	0.45
1:L:210:GLU:OE1	1:L:211:SER:N	2.45	0.45
1:L:265:LEU:O	1:L:266:PHE:C	2.60	0.45
1:L:480:GLU:C	1:L:482:PRO:HD2	2.41	0.45
1:L:359:VAL:O	1:L:360:GLU:C	2.59	0.45
1:L:462:ILE:O	1:L:465:ARG:N	2.45	0.45
1:L:498:LEU:O	1:L:500:TYR:N	2.49	0.45
1:L:129:LEU:CD1	1:L:164:MET:HG3	2.34	0.45
1:L:222:LEU:HD23	1:L:222:LEU:HA	1.60	0.45
1:L:487:LEU:HD23	1:L:487:LEU:N	2.32	0.45
1:L:127:LEU:HD23	1:L:168:VAL:HA	1.99	0.44
1:L:501:MET:CE	1:L:501:MET:CA	2.77	0.44
1:L:390:GLN:HB2	2:R:6:A:O3'	2.16	0.44
1:L:430:GLU:OE1	1:L:488:ARG:HD2	2.17	0.44
1:L:206:LEU:HD11	1:L:208:HIS:N	2.32	0.44
1:L:426:LEU:O	1:L:427:ILE:C	2.58	0.44
1:L:481:THR:N	1:L:482:PRO:HD2	2.33	0.44
1:L:26:ASP:OD1	1:L:27:LEU:N	2.49	0.44
1:L:221:TYR:CE2	1:L:371:ARG:HG3	2.52	0.44
1:L:222:LEU:HD21	1:L:226:ILE:HG21	1.99	0.44
1:L:250:PRO:C	1:L:252:PHE:N	2.76	0.44
1:L:299:LEU:HD12	1:L:299:LEU:N	2.32	0.44
1:L:423:ILE:CD1	1:L:484:TYR:CG	3.01	0.44
1:L:502:LEU:HA	1:L:502:LEU:HD23	1.00	0.44
1:L:4:MET:HE3	1:L:18:LEU:HD21	1.98	0.44
1:L:40:ASN:HD21	1:L:209:GLN:NE2	2.15	0.44
1:L:179:ALA:O	1:L:183:ASP:N	2.49	0.44
1:L:224:GLN:NE2	1:L:224:GLN:CA	2.77	0.44
1:L:362:ARG:HD2	1:L:362:ARG:C	2.43	0.44
1:L:367:VAL:HG23	1:L:370:ASP:HB2	2.00	0.44
1:L:419:LEU:HD12	1:L:423:ILE:HG12	1.99	0.44
1:L:265:LEU:HD21	1:L:269:TYR:CD1	2.51	0.44
1:L:498:LEU:O	1:L:501:MET:N	2.48	0.44
1:L:421:LEU:HD23	1:L:421:LEU:HA	1.49	0.43
1:L:222:LEU:CA	1:L:226:ILE:HD12	2.45	0.43
1:L:213:VAL:HG23	1:L:216:ARG:NH2	2.33	0.43
1:L:250:PRO:CD	1:L:251:ASP:H	2.31	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:445:VAL:HG12	1:L:446:PRO:HD3	1.96	0.43
1:L:24:LEU:HD21	1:L:336:LEU:HD21	2.00	0.43
1:L:352:PRO:HG2	1:L:355:HIS:CG	2.53	0.43
1:L:8:ALA:HB3	1:L:233:ASN:HB3	2.01	0.43
1:L:361:ASN:O	1:L:364:ARG:N	2.52	0.43
1:L:117:THR:HG1	1:L:119:PHE:HB2	1.79	0.43
1:L:280:GLN:HE21	1:L:280:GLN:HB2	1.69	0.43
1:L:304:ILE:O	1:L:305:ASN:HB3	2.19	0.43
1:L:286:PRO:O	1:L:287:SER:C	2.62	0.43
1:L:304:ILE:HG12	1:L:326:ALA:CB	2.48	0.43
1:L:51:PRO:C	1:L:53:LEU:N	2.75	0.43
1:L:432:LEU:O	1:L:433:LYS:C	2.62	0.42
1:L:434:GLU:O	1:L:435:ASN:HB2	2.18	0.42
1:L:120:ILE:HG22	1:L:122:LEU:CD1	2.49	0.42
1:L:268:HIS:C	1:L:270:GLN:H	2.27	0.42
1:L:433:LYS:O	1:L:436:THR:OG1	2.34	0.42
1:L:167:ILE:HG22	1:L:168:VAL:N	2.34	0.42
1:L:55:ALA:HB1	1:L:69:PRO:N	2.34	0.42
1:L:458:ALA:C	1:L:460:ASN:N	2.76	0.42
2:R:1:A:H8	2:R:2:C:H5	1.67	0.42
1:L:4:MET:HG3	1:L:18:LEU:HD23	2.01	0.42
1:L:37:LYS:O	1:L:40:ASN:OD1	2.38	0.42
1:L:205:PHE:HD1	1:L:206:LEU:O	1.94	0.42
1:L:120:ILE:CD1	1:L:120:ILE:H	2.32	0.42
1:L:304:ILE:CD1	1:L:326:ALA:HB1	2.49	0.42
1:L:357:ARG:HD3	1:L:357:ARG:HA	1.57	0.42
1:L:58:VAL:HB	1:L:116:LEU:CD1	2.49	0.42
1:L:282:GLU:C	1:L:283:VAL:CG2	2.92	0.42
1:L:285:LEU:HD11	1:L:326:ALA:HB2	2.01	0.42
1:L:422:SER:C	1:L:424:LEU:N	2.78	0.42
1:L:156:ALA:C	1:L:158:LEU:H	2.27	0.42
1:L:497:THR:HG22	1:L:502:LEU:HD21	2.01	0.42
1:L:102:VAL:CG1	1:L:116:LEU:HB3	2.50	0.41
1:L:502:LEU:CB	1:L:503:PRO:HD2	2.50	0.41
1:L:280:GLN:NE2	1:L:282:GLU:O	2.53	0.41
1:L:342:LEU:O	1:L:343:ILE:HG13	2.19	0.41
1:L:452:LEU:HA	1:L:452:LEU:HD23	1.75	0.41
1:L:90:ILE:O	1:L:93:VAL:N	2.52	0.41
1:L:139:ILE:HG22	1:L:140:SER:N	2.35	0.41
1:L:325:GLU:O	1:L:326:ALA:C	2.62	0.41
1:L:466:GLN:CD	1:L:466:GLN:N	2.77	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:64:ARG:O	1:L:65:HIS:C	2.64	0.41
1:L:190:HIS:C	1:L:192:GLU:N	2.78	0.41
1:L:258:LEU:C	1:L:258:LEU:HD23	2.46	0.41
1:L:453:ASN:O	1:L:456:ARG:N	2.49	0.41
1:L:490:ARG:C	1:L:491:LYS:O	2.62	0.41
1:L:132:ASN:N	1:L:164:MET:HB2	2.35	0.41
1:L:300:THR:O	1:L:343:ILE:HA	2.21	0.41
1:L:347:PHE:O	1:L:348:ILE:C	2.53	0.41
1:L:357:ARG:NH1	1:L:360:GLU:CD	2.79	0.41
1:L:498:LEU:N	1:L:498:LEU:HD23	2.35	0.41
1:L:183:ASP:O	1:L:186:PHE:N	2.54	0.41
1:L:211:SER:O	1:L:216:ARG:HG3	2.20	0.41
1:L:337:ARG:C	1:L:339:LEU:N	2.75	0.41
1:L:443:VAL:HB	1:L:444:PRO:HD2	2.02	0.41
1:L:7:ASN:HD21	1:L:9:THR:CG2	2.33	0.41
1:L:12:GLU:CD	1:L:12:GLU:H	2.29	0.41
1:L:14:LEU:O	1:L:14:LEU:HG	2.19	0.41
1:L:31:SER:C	1:L:32:PRO:O	2.63	0.41
1:L:206:LEU:CD1	1:L:208:HIS:N	2.83	0.41
1:L:233:ASN:HA	1:L:234:PRO:HD3	1.80	0.41
1:L:154:ALA:HB1	1:L:177:ALA:CB	2.48	0.41
1:L:281:ARG:NH1	1:L:292:VAL:HG11	2.36	0.41
1:L:320:PHE:CD1	1:L:355:HIS:CD2	3.09	0.41
1:L:15:ARG:HG2	1:L:29:ILE:HG13	2.02	0.40
1:L:268:HIS:C	1:L:270:GLN:N	2.79	0.40
1:L:372:ALA:CB	1:L:390:GLN:HG2	2.48	0.40
1:L:1:MET:HE1	1:L:228:GLU:CG	2.34	0.40
1:L:117:THR:C	1:L:119:PHE:N	2.78	0.40
1:L:131:PRO:CA	1:L:164:MET:HB2	2.52	0.40
1:L:156:ALA:C	1:L:158:LEU:N	2.77	0.40
1:L:424:LEU:HB2	1:L:451:LEU:HD21	2.04	0.40
2:R:5:U:H5	2:R:6:A:C2	2.40	0.40
1:L:103:GLN:O	1:L:117:THR:N	2.51	0.40
1:L:143:ILE:HG23	1:L:173:VAL:HG21	2.04	0.40
1:L:169:ARG:CG	1:L:169:ARG:NH1	2.38	0.40
1:L:206:LEU:CG	1:L:207:ILE:N	2.82	0.40
1:L:437:GLN:HA	1:L:437:GLN:NE2	2.37	0.40
1:L:109:ARG:HG2	1:L:109:ARG:HH21	1.86	0.40
1:L:214:ILE:HG23	1:L:218:PHE:CE1	2.55	0.40
1:L:299:LEU:HD22	1:L:344:VAL:HG23	2.02	0.40
1:L:330:ILE:O	1:L:331:ALA:C	2.63	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:498:LEU:CD1	1:L:500:TYR:CE2	3.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	L	337/439 (77%)	207 (61%)	130 (39%)	0 1

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	-4	ILE
1	L	3	ARG
1	L	9	THR
1	L	10	GLN
1	L	12	GLU
1	L	18	LEU
1	L	20	ASP
1	L	22	GLN
1	L	23	ARG
1	L	24	LEU
1	L	27	LEU
1	L	29	ILE
1	L	30	GLU
1	L	41	ILE
1	L	42	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	47	THR
1	L	52	SER
1	L	58	VAL
1	L	59	ASP
1	L	60	TYR
1	L	68	LEU
1	L	96	GLU
1	L	100	VAL
1	L	102	VAL
1	L	117	THR
1	L	118	THR
1	L	120	ILE
1	L	121	SER
1	L	122	LEU
1	L	125	SER
1	L	126	TYR
1	L	128	VAL
1	L	133	ASN
1	L	139	ILE
1	L	143	ILE
1	L	164	MET
1	L	166	LEU
1	L	167	ILE
1	L	168	VAL
1	L	169	ARG
1	L	173	VAL
1	L	180	LEU
1	L	201	ARG
1	L	206	LEU
1	L	211	SER
1	L	213	VAL
1	L	214	ILE
1	L	215	VAL
1	L	223	ARG
1	L	224	GLN
1	L	225	ASP
1	L	229	ILE
1	L	230	LEU
1	L	231	ILE
1	L	233	ASN
1	L	238	GLU
1	L	239	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	253	SER
1	L	254	SER
1	L	256	ILE
1	L	263	ILE
1	L	267	SER
1	L	270	GLN
1	L	272	GLU
1	L	277	SER
1	L	280	GLN
1	L	283	VAL
1	L	290	SER
1	L	291	ILE
1	L	293	ILE
1	L	296	THR
1	L	297	GLU
1	L	299	LEU
1	L	300	THR
1	L	304	ILE
1	L	305	ASN
1	L	315	ILE
1	L	318	THR
1	L	321	ASN
1	L	322	THR
1	L	330	ILE
1	L	332	ARG
1	L	338	ASP
1	L	348	ILE
1	L	349	ASP
1	L	350	MET
1	L	353	VAL
1	L	354	ARG
1	L	357	ARG
1	L	364	ARG
1	L	367	VAL
1	L	371	ARG
1	L	374	ILE
1	L	376	ILE
1	L	385	LEU
1	L	386	GLU
1	L	389	ARG
1	L	390	GLN
1	L	392	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	403	VAL
1	L	406	ARG
1	L	410	THR
1	L	413	VAL
1	L	419	LEU
1	L	425	ARG
1	L	426	LEU
1	L	428	GLU
1	L	432	LEU
1	L	435	ASN
1	L	436	THR
1	L	439	VAL
1	L	443	VAL
1	L	445	VAL
1	L	447	ILE
1	L	459	VAL
1	L	463	GLU
1	L	466	GLN
1	L	472	VAL
1	L	473	ILE
1	L	474	VAL
1	L	476	ASN
1	L	477	ASP
1	L	487	LEU
1	L	488	ARG
1	L	489	VAL
1	L	495	THR
1	L	497	THR
1	L	498	LEU
1	L	501	MET
1	L	502	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	7	ASN
1	L	22	GLN
1	L	40	ASN
1	L	132	ASN
1	L	133	ASN
1	L	224	GLN
1	L	233	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	305	ASN
1	L	355	HIS
1	L	356	GLN
1	L	416	ASN
1	L	437	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	R	10/10 (100%)	8 (80%)	7 (70%)

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	R	2	C
2	R	3	A
2	R	4	G
2	R	5	U
2	R	6	A
2	R	7	U
2	R	8	U
2	R	10	G

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	R	1	A
2	R	2	C
2	R	3	A
2	R	4	G
2	R	5	U
2	R	6	A
2	R	7	U

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	407:CYS	C	408:SER	N	1.17

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	L	491/517 (94%)	0.44	22 (4%) 38 21	21, 66, 85, 85	0
2	R	10/10 (100%)	0.73	1 (10%) 12 10	59, 79, 85, 85	0
All	All	501/527 (95%)	0.44	23 (4%) 37 21	21, 67, 85, 85	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	136	ALA	4.1
1	L	56	ALA	3.8
1	L	503	PRO	3.7
1	L	408	SER	3.7
1	L	79	PRO	3.6
1	L	246	ALA	3.3
1	L	90	ILE	3.0
1	L	67	PHE	2.9
1	L	416	ASN	2.9
1	L	349	ASP	2.7
1	L	491	LYS	2.4
1	L	36	GLN	2.4
1	L	455	LYS	2.4
1	L	135	ARG	2.3
1	L	471	CYS	2.3
2	R	10	G	2.2
1	L	469	VAL	2.2
1	L	475	PRO	2.1
1	L	467	ASP	2.1
1	L	57	PHE	2.1
1	L	116	LEU	2.1
1	L	39	ALA	2.0
1	L	292	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 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
4	ZN	L	1512	1/1	0.94	0.14	85,85,85,85	1
3	MG	L	1510	1/1	0.98	0.60	48,48,48,48	1
3	MG	L	1511	1/1	0.99	0.23	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.