



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:24 AM UTC

PDB ID : 1EIY / pdb_00001eiy
Title : THE CRYSTAL STRUCTURE OF PHENYLALANYL-TRNA SYN-
THETASE FROM THERMUS THERMOPHILUS COMPLEXED WITH
COGNATE TRNAPHE
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Deposited on : 2000-02-29
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 : 4-5-2 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

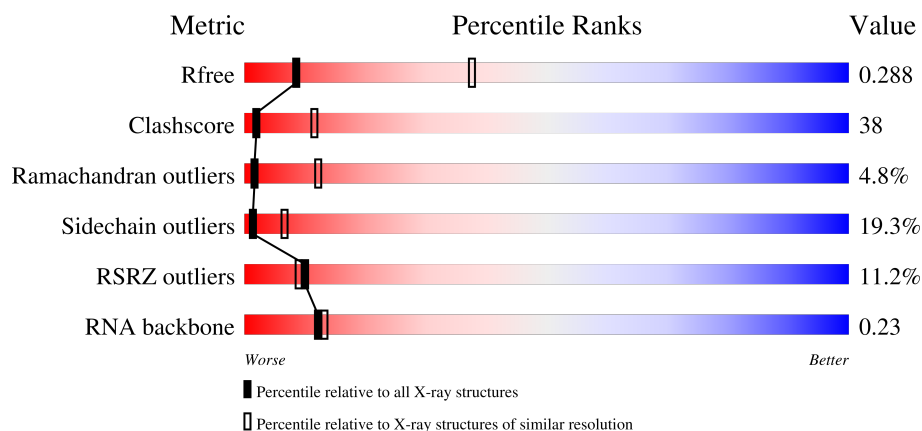
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

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	C	76	88% 7% 42% 36% 16%
2	A	350	14% 32% 47% 18% ..
3	B	785	2% 36% 44% 18% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10485 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(PHE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	76	Total	C	N	O	P	0	0	0
			1623	723	291	533	76			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	49	C	G	conflict	UNP Q5SGX1
C	65	G	C	conflict	UNP Q5SGX1

- Molecule 2 is a protein called PHENYLALANYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	345	Total	C	N	O	S	0	0	0
			2735	1768	477	482	8			

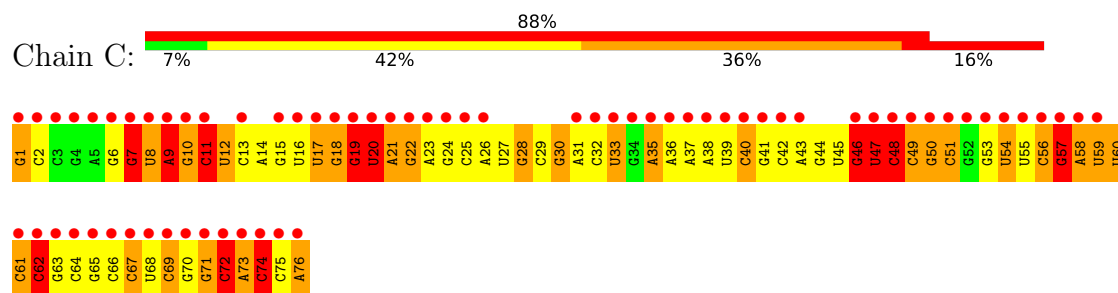
- Molecule 3 is a protein called PHENYLALANYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	785	Total	C	N	O	S	0	0	0
			6127	3925	1091	1101	10			

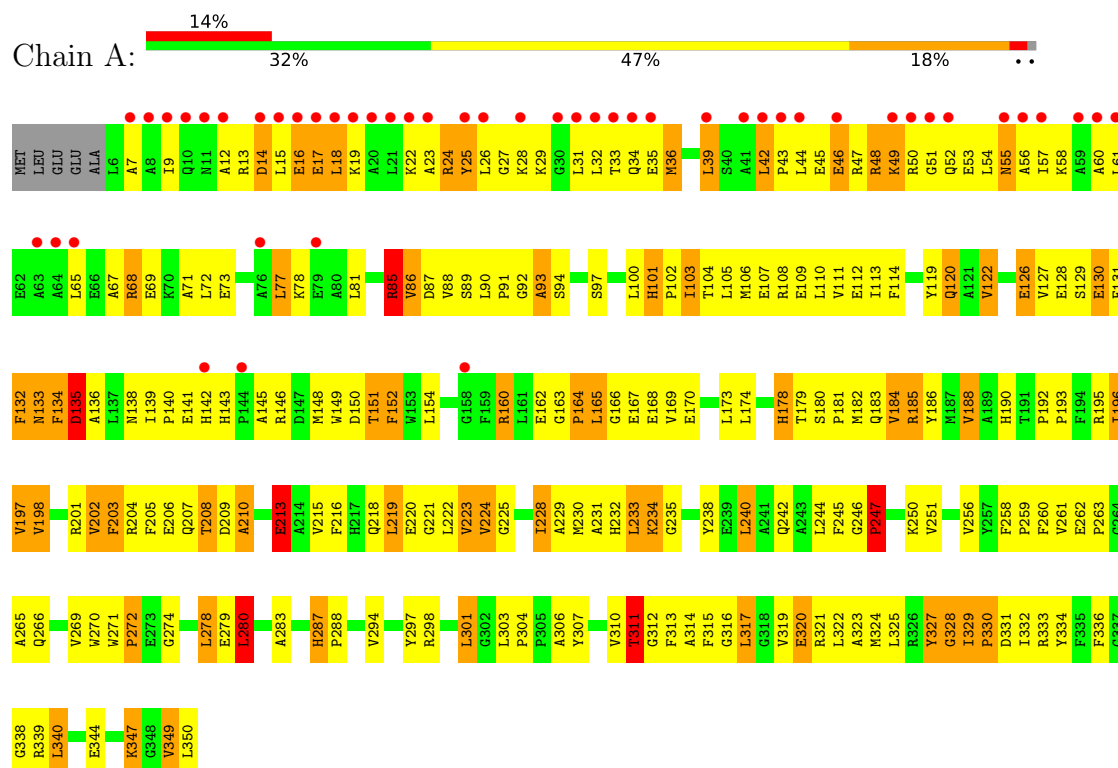
3 Residue-property plots [i](#)

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(PHE)

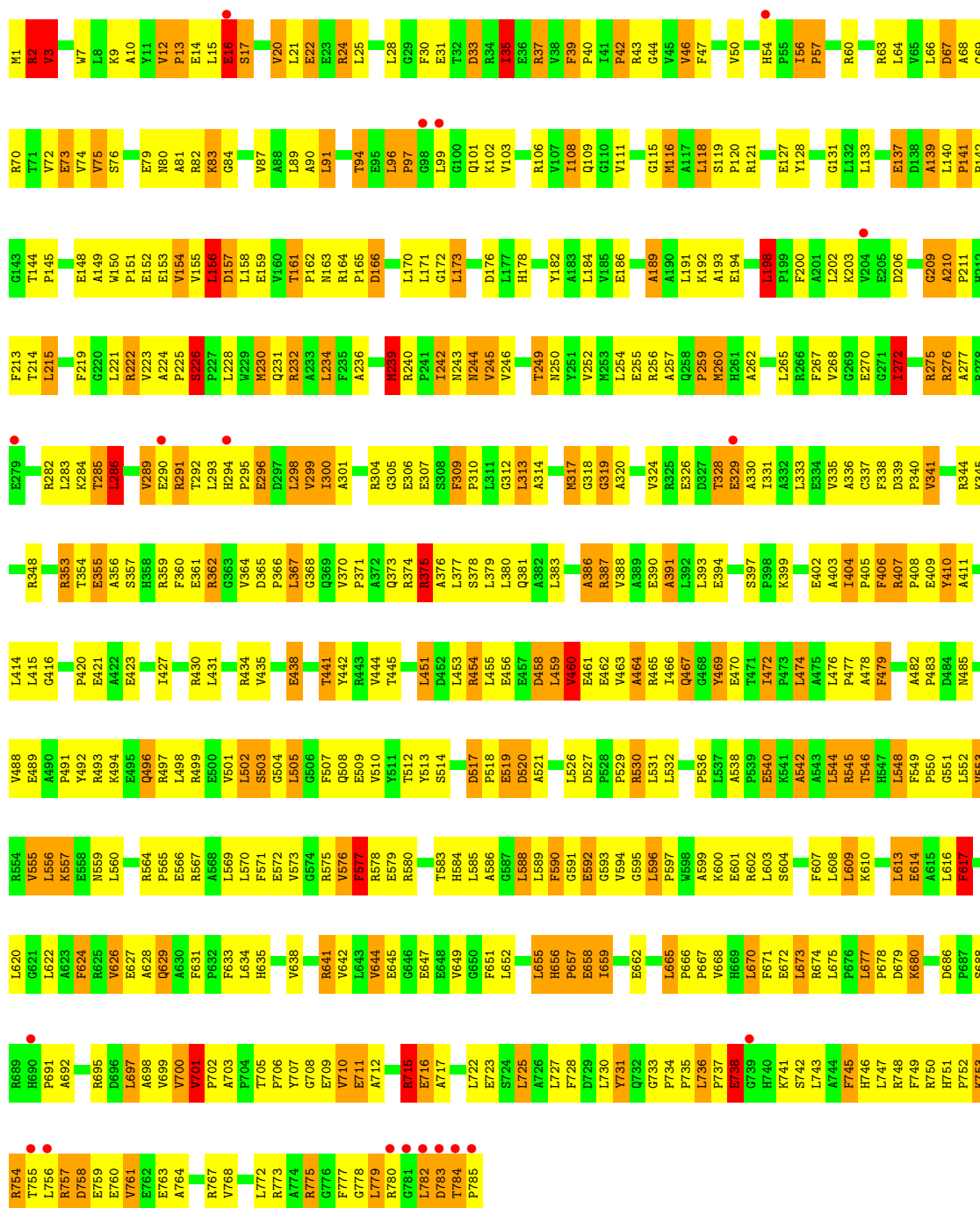


• Molecule 2: PHENYLALANYL-TRNA SYNTHETASE



• Molecule 3: PHENYLALANYL-TRNA SYNTHETASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	175.00Å 175.00Å 140.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.00 – 3.30 28.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	86.3 (28.00-3.30) 87.8 (28.00-3.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.30 (at 3.31Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.221 , 0.287 0.236 , 0.288	Depositor DCC
R_{free} test set	1657 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	59.2	Xtriage
Anisotropy	0.685	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 75.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.080 for -h,-k,l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	10485	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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

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	C	0.68	1/1813 (0.1%)	1.11	16/2823 (0.6%)
2	A	1.12	2/2805 (0.1%)	1.52	47/3789 (1.2%)
3	B	1.03	9/6280 (0.1%)	1.52	120/8536 (1.4%)
All	All	1.00	12/10898 (0.1%)	1.45	183/15148 (1.2%)

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	C	0	6
3	B	0	1
All	All	0	7

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	239	MET	SD-CE	12.98	2.12	1.79
3	B	249	THR	CA-CB	7.45	1.65	1.53
2	A	197	VAL	CA-CB	7.00	1.63	1.54
3	B	460	VAL	CA-CB	7.00	1.62	1.54
1	C	1	G	OP3-P	6.74	1.61	1.48
3	B	784	THR	CA-CB	6.71	1.64	1.53
3	B	784	THR	CA-C	5.89	1.60	1.52
3	B	259	PRO	CA-C	5.85	1.59	1.52
3	B	464	ALA	N-CA	-5.67	1.40	1.46
3	B	245	VAL	CA-CB	5.50	1.60	1.54
3	B	472	ILE	CA-CB	5.40	1.60	1.54
2	A	223	VAL	CA-CB	5.38	1.61	1.54

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	163	GLY	CA-C-N	11.49	134.20	119.84
2	A	163	GLY	C-N-CA	11.49	134.20	119.84
3	B	224	ALA	CA-C-N	-11.35	109.19	120.31
3	B	224	ALA	C-N-CA	-11.35	109.19	120.31
2	A	246	GLY	CA-C-N	11.30	133.96	119.84
2	A	246	GLY	C-N-CA	11.30	133.96	119.84
3	B	161	THR	CA-C-N	10.96	132.18	119.47
3	B	161	THR	C-N-CA	10.96	132.18	119.47
3	B	431	LEU	N-CA-C	-10.95	99.37	113.17
3	B	293	LEU	N-CA-C	10.85	124.85	110.53
3	B	783	ASP	N-CA-C	10.64	126.97	113.88
3	B	647	GLU	N-CA-C	10.41	126.93	110.17
3	B	96	LEU	CA-C-N	10.01	132.35	119.84
3	B	96	LEU	C-N-CA	10.01	132.35	119.84
3	B	700	VAL	N-CA-C	9.90	120.72	110.72
3	B	466	ILE	N-CA-C	-9.83	101.29	110.53
2	A	151	THR	N-CA-C	9.71	125.20	109.76
3	B	472	ILE	N-CA-C	-9.67	96.94	107.77
3	B	339	ASP	CA-C-N	9.53	131.75	119.84
3	B	339	ASP	C-N-CA	9.53	131.75	119.84
2	A	169	VAL	N-CA-C	9.40	122.72	108.71
2	A	213	GLU	N-CA-C	9.32	123.05	108.79
3	B	56	ILE	N-CA-C	-9.24	98.40	107.55
2	A	329	ILE	CA-C-N	9.19	131.33	119.84
2	A	329	ILE	C-N-CA	9.19	131.33	119.84
2	A	25	TYR	N-CA-C	-9.10	101.94	113.23
3	B	68	ALA	N-CA-C	-9.06	98.77	111.81
3	B	309	PHE	CA-C-N	9.04	129.39	119.90
3	B	309	PHE	C-N-CA	9.04	129.39	119.90
3	B	442	TYR	N-CA-C	8.86	124.22	113.41
2	A	18	LEU	N-CA-C	-8.80	101.77	111.36
2	A	287	HIS	CA-C-N	8.61	129.14	119.32
2	A	287	HIS	C-N-CA	8.61	129.14	119.32
3	B	779	LEU	N-CA-C	8.58	121.39	109.29
1	C	19	G	C3'-C2'-O2'	8.39	123.29	110.70
3	B	469	TYR	N-CA-C	-8.35	102.98	113.01
1	C	20	U	C2'-C3'-O3'	8.20	126.00	113.70
3	B	56	ILE	CA-C-N	8.11	129.98	119.84
3	B	56	ILE	C-N-CA	8.11	129.98	119.84
3	B	577	PHE	N-CA-C	7.97	121.51	108.52
3	B	715	ARG	N-CA-C	7.97	119.96	111.28
3	B	596	LEU	CA-C-N	7.53	127.06	118.85
3	B	596	LEU	C-N-CA	7.53	127.06	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	545	ARG	N-CA-C	7.46	121.08	109.96
3	B	30	PHE	N-CA-C	7.40	120.85	108.20
3	B	658	GLU	N-CA-C	-7.37	102.94	110.97
2	A	280	LEU	N-CA-C	7.37	126.49	110.80
3	B	37	ARG	N-CA-C	-7.35	97.71	109.76
3	B	16	GLU	N-CA-C	7.32	126.39	110.80
3	B	527	ASP	CA-C-N	7.18	127.77	120.38
3	B	527	ASP	C-N-CA	7.18	127.77	120.38
3	B	745	PHE	N-CA-C	7.09	119.97	108.41
2	A	152	PHE	N-CA-C	-6.97	97.87	108.67
3	B	383	LEU	N-CA-C	6.79	119.54	111.33
2	A	203	PHE	N-CA-C	6.73	119.37	108.34
3	B	141	PRO	CA-C-N	6.63	128.12	119.84
3	B	141	PRO	C-N-CA	6.63	128.12	119.84
2	A	225	GLY	N-CA-C	-6.57	101.10	110.63
2	A	173	LEU	N-CA-C	6.50	119.90	110.28
3	B	601	GLU	N-CA-C	6.48	119.81	109.24
3	B	560	LEU	N-CA-C	-6.48	104.14	111.14
3	B	387	ARG	N-CA-C	-6.47	98.69	109.24
2	A	207	GLN	N-CA-C	6.43	119.74	108.56
3	B	677	LEU	N-CA-C	-6.43	99.58	109.41
2	A	14	ASP	N-CA-C	-6.42	103.53	112.45
3	B	166	ASP	N-CA-C	-6.41	105.28	113.23
3	B	761	VAL	N-CA-C	-6.40	104.26	110.72
3	B	504	GLY	N-CA-C	-6.36	104.91	113.24
3	B	300	ILE	N-CA-C	-6.31	98.11	107.51
1	C	56	C	N1-C1'-C2'	6.30	121.46	112.00
3	B	410	TYR	N-CA-C	-6.28	104.51	111.36
3	B	438	GLU	N-CA-C	-6.28	105.75	113.41
1	C	47	U	N1-C1'-C2'	6.25	121.38	112.00
3	B	35	ILE	N-CA-C	-6.21	99.29	108.85
3	B	379	LEU	N-CA-C	-6.20	104.21	110.97
3	B	603	LEU	N-CA-C	-6.19	97.98	108.26
3	B	624	PHE	N-CA-C	6.15	118.42	108.34
2	A	44	LEU	N-CA-C	-6.08	106.40	113.88
3	B	697	LEU	N-CA-C	6.07	116.44	107.88
3	B	701	VAL	CA-C-N	6.06	127.41	119.84
3	B	701	VAL	C-N-CA	6.06	127.41	119.84
2	A	334	TYR	N-CA-C	6.01	121.29	111.37
3	B	701	VAL	N-CA-C	5.93	121.69	108.88
3	B	458	ASP	N-CA-C	-5.93	104.94	111.82
3	B	617	PHE	N-CA-C	5.91	118.21	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	553	VAL	CB-CA-C	-5.88	104.10	112.22
2	A	154	LEU	N-CA-C	5.86	119.51	110.42
2	A	234	LYS	N-CA-C	-5.86	104.90	111.28
1	C	74	C	C4'-C3'-O3'	5.85	121.78	113.00
3	B	119	SER	N-CA-C	-5.80	103.46	110.13
3	B	731	TYR	N-CA-C	5.80	118.95	108.69
2	A	24	ARG	N-CA-C	5.79	120.51	113.38
3	B	54	HIS	CA-C-N	-5.76	114.03	119.85
3	B	54	HIS	C-N-CA	-5.76	114.03	119.85
3	B	232	ARG	CA-C-N	5.75	128.25	120.44
3	B	232	ARG	C-N-CA	5.75	128.25	120.44
3	B	154	VAL	N-CA-C	-5.74	100.13	108.17
3	B	231	GLN	N-CA-C	-5.73	104.64	111.69
3	B	286	LEU	N-CA-C	5.72	122.99	110.80
3	B	656	HIS	CA-C-N	5.72	126.99	119.84
3	B	656	HIS	C-N-CA	5.72	126.99	119.84
1	C	28	G	C3'-C2'-O2'	5.71	119.26	110.70
3	B	210	ALA	CA-C-N	5.70	125.82	119.32
3	B	210	ALA	C-N-CA	5.70	125.82	119.32
3	B	670	LEU	N-CA-C	5.70	117.44	108.96
3	B	542	ALA	N-CA-C	5.68	120.21	112.04
2	A	208	THR	N-CA-C	5.67	122.88	110.80
3	B	3	VAL	N-CA-C	5.65	121.08	108.88
3	B	727	LEU	N-CA-C	-5.63	101.51	109.96
3	B	517	ASP	N-CA-C	-5.62	102.70	109.72
3	B	156	LEU	N-CA-C	5.61	118.05	108.90
3	B	520	ASP	N-CA-C	5.61	118.93	111.75
3	B	710	VAL	N-CA-C	-5.61	105.04	110.42
2	A	223	VAL	N-CA-C	-5.58	97.73	109.34
2	A	86	VAL	N-CA-C	5.58	116.13	110.05
3	B	626	VAL	N-CA-C	-5.57	99.62	107.75
2	A	231	ALA	CA-C-N	5.54	128.16	120.29
2	A	231	ALA	C-N-CA	5.54	128.16	120.29
1	C	46	G	N9-C1'-C2'	5.54	120.32	112.00
2	A	16	GLU	N-CA-C	-5.54	105.64	112.90
3	B	355	GLU	N-CA-C	-5.54	105.34	111.71
3	B	189	ALA	N-CA-C	-5.54	96.71	107.62
2	A	85	ARG	N-CA-C	-5.53	99.02	110.80
2	A	210	ALA	N-CA-C	5.53	118.07	111.71
3	B	328	THR	N-CA-C	-5.51	102.33	110.48
1	C	46	G	C4'-C3'-O3'	-5.50	104.75	113.00
2	A	39	LEU	N-CA-C	-5.50	103.14	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	11	C	N1-C1'-C2'	5.49	120.23	112.00
2	A	233	LEU	N-CA-C	-5.49	105.38	111.36
3	B	262	ALA	N-CA-C	-5.48	100.24	109.07
3	B	627	GLU	N-CA-C	-5.46	101.26	109.95
2	A	17	GLU	N-CA-C	-5.43	105.91	112.54
2	A	135	ASP	N-CA-C	-5.42	99.25	110.80
3	B	375	ARG	CA-C-N	5.41	127.48	120.44
3	B	375	ARG	C-N-CA	5.41	127.48	120.44
3	B	711	GLU	N-CA-C	5.40	117.87	111.33
3	B	225	PRO	N-CA-C	-5.39	103.37	111.57
3	B	226	SER	CA-C-N	5.38	125.38	119.89
3	B	226	SER	C-N-CA	5.38	125.38	119.89
3	B	22	GLU	CA-C-N	5.38	127.75	120.44
3	B	22	GLU	C-N-CA	5.38	127.75	120.44
1	C	62	C	N1-C1'-C2'	-5.37	103.95	112.00
1	C	74	C	O4'-C4'-C3'	-5.36	98.64	104.00
3	B	198	LEU	N-CA-C	-5.36	102.90	109.65
1	C	71	G	N9-C1'-C2'	-5.35	103.97	112.00
3	B	416	GLY	N-CA-C	-5.34	107.87	115.30
3	B	460	VAL	N-CA-CB	5.34	116.80	110.55
3	B	435	VAL	CB-CA-C	-5.34	105.83	112.45
2	A	60	ALA	N-CA-C	-5.33	105.14	111.69
3	B	2	ARG	N-CA-C	-5.32	99.46	110.80
3	B	736	LEU	CA-C-N	5.31	126.48	119.84
3	B	736	LEU	C-N-CA	5.31	126.48	119.84
3	B	13	PRO	N-CA-C	-5.31	101.86	110.40
3	B	644	VAL	CB-CA-C	-5.30	103.95	111.21
1	C	9	A	C2'-C3'-O3'	5.30	117.45	109.50
3	B	479	PHE	N-CA-C	5.30	116.57	108.52
3	B	592	GLU	N-CA-C	5.25	117.08	111.36
2	A	46	GLU	N-CA-C	5.24	121.97	110.80
3	B	546	THR	N-CA-C	-5.21	106.92	113.28
3	B	118	LEU	N-CA-C	5.18	118.51	110.17
2	A	247	PRO	N-CA-C	5.17	123.11	112.47
3	B	782	LEU	N-CA-C	5.16	120.04	113.18
3	B	407	ARG	N-CA-C	-5.15	99.26	109.10
2	A	101	HIS	N-CA-C	-5.15	102.55	110.32
2	A	198	VAL	CA-C-N	5.13	126.98	120.51
2	A	198	VAL	C-N-CA	5.13	126.98	120.51
3	B	717	ALA	N-CA-C	-5.13	107.19	113.50
1	C	20	U	C5'-C4'-C3'	-5.11	108.33	116.00
3	B	665	LEU	CA-C-N	5.11	125.64	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	665	LEU	C-N-CA	5.11	125.64	120.38
3	B	299	VAL	N-CA-C	5.10	117.17	108.86
3	B	445	THR	CA-C-N	5.09	123.32	119.66
3	B	445	THR	C-N-CA	5.09	123.32	119.66
3	B	228	LEU	N-CA-C	5.09	117.23	111.02
3	B	230	MET	CB-CG-SD	5.08	127.94	112.70
1	C	7	G	C2'-C3'-O3'	5.07	117.11	109.50
3	B	686	ASP	N-CA-C	-5.05	103.67	109.93
2	A	311	THR	N-CA-C	-5.04	102.33	110.14
2	A	216	PHE	N-CA-C	5.04	115.96	108.60
1	C	72	C	C2'-C3'-O3'	-5.03	106.15	113.70
2	A	347	LYS	N-CA-C	-5.02	106.00	111.82
3	B	272	ILE	CB-CA-C	-5.02	104.11	110.98
2	A	7	ALA	N-CA-C	5.01	121.48	110.80

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	617	PHE	Sidechain
1	C	19	G	Sidechain
1	C	30	G	Sidechain
1	C	48	C	Sidechain
1	C	57	G	Sidechain
1	C	60	U	Sidechain
1	C	62	C	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1623	0	822	133	0
2	A	2735	0	2725	249	0
3	B	6127	0	6180	435	0
All	All	10485	0	9727	777	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 38.

All (777) 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)
3:B:239:MET:CE	3:B:239:MET:SD	2.12	1.38
1:C:58:A:H4'	1:C:59:U:OP1	1.41	1.17
3:B:706:PRO:HG2	3:B:709:GLU:HB2	1.29	1.08
1:C:39:U:C2'	1:C:40:C:H5'	1.83	1.07
1:C:39:U:H2'	1:C:40:C:H5'	1.38	1.02
2:A:210:ALA:HA	2:A:331:ASP:HB2	1.38	1.02
1:C:47:U:H3'	1:C:48:C:H5'	1.38	1.01
1:C:8:U:H4'	1:C:48:C:H1'	1.42	1.01
2:A:23:ALA:HB2	2:A:65:LEU:HD21	1.40	1.01
3:B:282:ARG:HD2	3:B:292:THR:HG22	1.43	1.01
2:A:19:LYS:HD3	2:A:22:LYS:HD2	1.43	1.00
3:B:314:ALA:HB1	3:B:338:PHE:HE1	1.25	0.99
2:A:12:ALA:HA	2:A:15:LEU:HB3	1.46	0.95
3:B:221:LEU:HD23	3:B:386:ALA:HB2	1.46	0.95
3:B:12:VAL:HG22	3:B:15:LEU:HD13	1.50	0.94
1:C:61:C:H2'	1:C:62:C:C6	2.03	0.93
1:C:53:G:H2'	1:C:54:U:C6	2.05	0.90
1:C:61:C:H2'	1:C:62:C:H6	1.36	0.90
2:A:119:TYR:HD2	2:A:197:VAL:HG13	1.37	0.89
2:A:294:VAL:O	2:A:298:ARG:HG3	1.73	0.89
3:B:312:GLY:HA2	3:B:318:GLY:HA2	1.53	0.88
2:A:183:GLN:HG3	2:A:222:LEU:HD22	1.56	0.88
3:B:285:THR:HG21	3:B:291:ARG:HE	1.39	0.88
3:B:163:ASN:O	3:B:165:PRO:HD3	1.74	0.87
3:B:162:PRO:HA	3:B:362:ARG:HD3	1.55	0.86
1:C:8:U:C4'	1:C:48:C:H1'	2.06	0.85
1:C:55:U:H3'	1:C:55:U:C6	2.12	0.85
1:C:65:G:C2'	1:C:66:C:H5'	2.06	0.85
2:A:26:LEU:HD22	2:A:61:LEU:HD21	1.60	0.84
3:B:314:ALA:HB1	3:B:338:PHE:CE1	2.11	0.84
1:C:65:G:H2'	1:C:66:C:H5'	1.58	0.83
1:C:41:G:O2'	1:C:42:C:H5'	1.77	0.83
2:A:42:LEU:H	2:A:43:PRO:HD2	1.42	0.83
3:B:609:LEU:CD1	3:B:652:LEU:HD11	2.08	0.83
2:A:179:THR:OG1	2:A:220:GLU:HG3	1.77	0.82
2:A:287:HIS:CD2	2:A:288:PRO:HD2	2.13	0.82
1:C:53:G:H2'	1:C:54:U:H6	1.43	0.82
3:B:336:ALA:HB3	3:B:338:PHE:HE2	1.40	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:453:LEU:HD23	3:B:458:ASP:HB3	1.60	0.82
3:B:286:LEU:HD23	3:B:317:MET:HE1	1.62	0.82
2:A:265:ALA:HB2	3:B:469:TYR:HE1	1.43	0.81
3:B:549:PHE:O	3:B:553:VAL:HG23	1.79	0.81
3:B:734:PRO:HA	3:B:736:LEU:H	1.43	0.81
1:C:9:A:N6	1:C:23:A:H62	1.79	0.80
3:B:734:PRO:HA	3:B:736:LEU:N	1.97	0.80
3:B:609:LEU:HD13	3:B:652:LEU:HD11	1.64	0.80
3:B:505:LEU:HD12	3:B:507:PHE:HE1	1.47	0.80
1:C:47:U:H3'	1:C:48:C:C5'	2.12	0.79
1:C:31:A:O2'	1:C:32:C:H5'	1.82	0.79
3:B:283:LEU:HD21	3:B:320:ALA:HB2	1.63	0.79
1:C:31:A:C2'	1:C:32:C:H5'	2.11	0.79
2:A:19:LYS:HG3	2:A:68:ARG:HG2	1.63	0.79
2:A:91:PRO:HB2	3:B:597:PRO:HG3	1.64	0.78
3:B:733:GLY:O	3:B:736:LEU:HB2	1.81	0.78
1:C:9:A:H4'	1:C:10:G:OP1	1.82	0.78
2:A:18:LEU:O	2:A:22:LYS:HG3	1.84	0.78
2:A:164:PRO:HB2	2:A:165:LEU:HD23	1.64	0.78
3:B:284:LYS:O	3:B:320:ALA:HA	1.82	0.78
3:B:221:LEU:CD2	3:B:386:ALA:HB2	2.14	0.78
2:A:85:ARG:HG3	2:A:85:ARG:HH11	1.46	0.77
3:B:589:LEU:CD2	3:B:609:LEU:HB2	2.13	0.77
1:C:72:C:H5''	1:C:73:A:OP2	1.83	0.77
1:C:63:G:H2'	1:C:64:C:C6	2.19	0.77
3:B:589:LEU:HD22	3:B:609:LEU:HB2	1.66	0.77
3:B:501:VAL:O	3:B:505:LEU:HB2	1.86	0.76
3:B:557:LYS:HG2	3:B:665:LEU:HD23	1.67	0.76
3:B:730:LEU:HD12	3:B:743:LEU:CD2	2.16	0.76
1:C:9:A:N6	1:C:22:G:C5	2.53	0.75
1:C:61:C:C5	1:C:62:C:C5	2.74	0.75
1:C:47:U:H2'	1:C:50:G:OP1	1.86	0.75
1:C:75:C:OP1	3:B:159:GLU:HG3	1.87	0.75
1:C:65:G:O2'	1:C:66:C:H5'	1.87	0.74
2:A:265:ALA:HB2	3:B:469:TYR:CE1	2.21	0.74
3:B:191:LEU:HB2	3:B:381:GLN:NE2	2.01	0.74
2:A:321:ARG:O	2:A:325:LEU:HD23	1.87	0.74
1:C:14:A:H2'	1:C:15:G:H5'	1.69	0.74
2:A:51:GLY:HA2	2:A:55:ASN:ND2	2.03	0.73
3:B:312:GLY:CA	3:B:318:GLY:HA2	2.18	0.73
3:B:414:LEU:HD23	3:B:460:VAL:HG21	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:215:LEU:HD21	3:B:272:ILE:HG13	1.70	0.73
1:C:9:A:H62	1:C:23:A:N6	1.86	0.73
1:C:39:U:O2'	1:C:40:C:H5'	1.88	0.73
2:A:32:LEU:HA	2:A:36:MET:HG2	1.71	0.73
3:B:221:LEU:HD11	3:B:331:ILE:HG12	1.69	0.73
3:B:39:PHE:N	3:B:40:PRO:HD3	2.03	0.73
3:B:505:LEU:HD12	3:B:507:PHE:CE1	2.23	0.73
1:C:39:U:H2'	1:C:40:C:C5'	2.18	0.72
3:B:336:ALA:HB3	3:B:338:PHE:CE2	2.23	0.72
2:A:127:VAL:HG23	3:B:577:PHE:CE2	2.24	0.72
3:B:517:ASP:HB2	3:B:519:GLU:OE1	1.90	0.72
3:B:191:LEU:HB2	3:B:381:GLN:HE22	1.52	0.72
2:A:49:LYS:H	2:A:49:LYS:HD2	1.55	0.72
3:B:659:ILE:HA	3:B:662:GLU:HB3	1.72	0.71
3:B:604:SER:HA	3:B:608:LEU:HD22	1.72	0.71
2:A:109:GLU:O	2:A:113:ILE:HG13	1.91	0.70
3:B:715:ARG:HG3	3:B:725:LEU:HD22	1.72	0.70
3:B:755:THR:HG22	3:B:756:LEU:H	1.56	0.70
3:B:222:ARG:CG	3:B:222:ARG:HH11	2.03	0.70
3:B:286:LEU:HB2	3:B:319:GLY:HA3	1.73	0.70
2:A:35:GLU:O	2:A:39:LEU:HD23	1.91	0.70
3:B:198:LEU:HD11	3:B:391:ALA:O	1.91	0.70
1:C:61:C:C6	1:C:62:C:C5	2.80	0.70
3:B:355:GLU:O	3:B:359:ARG:HD3	1.91	0.70
2:A:107:GLU:O	2:A:111:VAL:HG23	1.92	0.69
3:B:588:LEU:HD12	3:B:668:VAL:HG11	1.71	0.69
1:C:55:U:C6	1:C:55:U:C3'	2.75	0.69
1:C:68:U:C2'	1:C:69:C:H5'	2.22	0.69
2:A:120:GLN:HB2	2:A:196:ILE:HG22	1.74	0.69
1:C:9:A:N6	1:C:23:A:N6	2.40	0.69
1:C:41:G:C2'	1:C:42:C:H5'	2.23	0.69
3:B:294:HIS:HD2	3:B:296:GLU:HB2	1.56	0.69
1:C:45:U:H3'	1:C:46:G:C5'	2.23	0.68
3:B:277:ALA:O	3:B:295:PRO:HA	1.93	0.68
3:B:96:LEU:HB2	3:B:99:LEU:HD13	1.73	0.68
1:C:24:G:C6	1:C:25:C:C2	2.80	0.68
2:A:102:PRO:HA	2:A:105:LEU:HD12	1.74	0.68
3:B:536:PRO:HB3	3:B:542:ALA:HA	1.76	0.68
2:A:13:ARG:NE	2:A:72:LEU:HD22	2.09	0.68
1:C:76:A:C8	2:A:149:TRP:CZ2	2.81	0.68
3:B:427:ILE:HG21	3:B:463:VAL:HA	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:U:H2'	1:C:35:A:OP2	1.94	0.68
3:B:624:PHE:HE2	3:B:642:VAL:HG13	1.58	0.68
3:B:13:PRO:O	3:B:14:GLU:HG2	1.94	0.68
2:A:101:HIS:CD2	2:A:103:ILE:H	2.12	0.68
2:A:129:SER:O	2:A:131:PHE:N	2.28	0.67
3:B:751:HIS:CD2	3:B:753:LYS:HB3	2.29	0.67
3:B:688:SER:HB3	3:B:752:PRO:HA	1.75	0.67
3:B:249:THR:HA	3:B:260:MET:CE	2.25	0.67
1:C:26:A:C2	1:C:27:U:C6	2.82	0.67
1:C:27:U:H2'	1:C:28:G:H8	1.59	0.67
2:A:51:GLY:HA2	2:A:55:ASN:HD21	1.60	0.67
3:B:213:PHE:HE2	3:B:215:LEU:HD13	1.59	0.67
3:B:16:GLU:O	3:B:17:SER:HB3	1.95	0.67
1:C:36:A:C2	1:C:37:A:C8	2.83	0.67
2:A:232:HIS:CD2	3:B:477:PRO:HB3	2.30	0.67
2:A:233:LEU:HD13	2:A:313:PHE:CD1	2.30	0.67
1:C:75:C:O2'	2:A:148:MET:HG2	1.95	0.67
3:B:368:GLY:O	3:B:371:PRO:HG2	1.95	0.67
3:B:701:VAL:HG23	3:B:705:THR:HG21	1.75	0.66
3:B:198:LEU:HD12	3:B:393:LEU:HD13	1.76	0.66
3:B:715:ARG:HG3	3:B:725:LEU:CD2	2.25	0.66
2:A:287:HIS:HD2	2:A:288:PRO:HD2	1.58	0.66
3:B:64:LEU:HD11	3:B:76:SER:HB3	1.76	0.66
1:C:54:U:H3'	1:C:58:A:H61	1.60	0.66
2:A:110:LEU:O	2:A:114:PHE:HD1	1.78	0.66
3:B:331:ILE:HD11	3:B:380:LEU:HD21	1.78	0.66
3:B:596:LEU:HB2	3:B:599:ALA:HB3	1.76	0.66
2:A:181:PRO:O	2:A:185:ARG:HG3	1.95	0.66
3:B:178:HIS:HD2	3:B:182:TYR:O	1.79	0.66
3:B:276:ARG:HH11	3:B:276:ARG:CG	2.09	0.65
1:C:65:G:H2'	1:C:66:C:C5'	2.27	0.65
3:B:282:ARG:CD	3:B:292:THR:HG22	2.25	0.65
2:A:126:GLU:HG2	2:A:203:PHE:HE1	1.61	0.65
2:A:210:ALA:CA	2:A:331:ASP:HB2	2.21	0.65
2:A:222:LEU:HD12	2:A:224:VAL:HG22	1.77	0.65
3:B:467:GLN:HE21	3:B:467:GLN:HA	1.61	0.65
3:B:376:ALA:O	3:B:380:LEU:HB2	1.97	0.65
1:C:14:A:C2'	1:C:15:G:H5'	2.27	0.65
3:B:189:ALA:HB1	3:B:378:SER:HB3	1.79	0.64
2:A:128:GLU:HG3	2:A:129:SER:H	1.62	0.64
2:A:19:LYS:HA	2:A:22:LYS:HB2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:751:HIS:HB3	3:B:754:ARG:O	1.97	0.64
2:A:73:GLU:O	2:A:77:LEU:HB3	1.97	0.64
3:B:120:PRO:HD2	3:B:128:TYR:O	1.97	0.64
2:A:119:TYR:CD2	2:A:197:VAL:HG13	2.26	0.64
3:B:219:PHE:HA	3:B:330:ALA:HA	1.80	0.64
1:C:31:A:H2'	1:C:32:C:H5'	1.78	0.64
1:C:68:U:H2'	1:C:69:C:H5'	1.80	0.63
3:B:407:ARG:HG2	3:B:441:THR:HG23	1.79	0.63
3:B:712:ALA:O	3:B:716:GLU:HG3	1.98	0.63
2:A:327:TYR:N	2:A:327:TYR:CD2	2.65	0.63
2:A:43:PRO:HA	2:A:50:ARG:NH1	2.13	0.63
2:A:234:LYS:HB3	3:B:474:LEU:HD22	1.80	0.63
3:B:353:ARG:N	3:B:353:ARG:HD3	2.14	0.63
3:B:404:ILE:HD13	3:B:454:ARG:O	1.99	0.63
3:B:624:PHE:CE2	3:B:642:VAL:HG13	2.33	0.63
3:B:698:ALA:HB3	3:B:780:ARG:CG	2.28	0.63
1:C:8:U:O2'	1:C:46:G:N2	2.32	0.63
3:B:344:ARG:O	3:B:348:ARG:HG3	1.98	0.63
3:B:569:LEU:HD13	3:B:589:LEU:HD13	1.81	0.63
3:B:284:LYS:HG3	3:B:289:VAL:O	1.99	0.62
2:A:297:TYR:CE1	2:A:301:LEU:HD11	2.34	0.62
2:A:195:ARG:HG2	2:A:223:VAL:HG22	1.81	0.62
3:B:14:GLU:O	3:B:14:GLU:HG3	1.99	0.62
2:A:279:GLU:O	2:A:280:LEU:HB2	2.00	0.62
3:B:453:LEU:CD2	3:B:458:ASP:HB3	2.29	0.62
3:B:120:PRO:HD3	3:B:131:GLY:O	1.99	0.62
2:A:87:ASP:HB3	2:A:90:LEU:HD22	1.82	0.62
2:A:182:MET:HE3	2:A:182:MET:O	2.00	0.62
3:B:779:LEU:H	3:B:783:ASP:HB2	1.64	0.62
1:C:55:U:H3'	1:C:55:U:H6	1.64	0.62
3:B:335:VAL:HB	3:B:373:GLN:HE21	1.63	0.62
2:A:32:LEU:CD2	2:A:36:MET:HE2	2.30	0.61
1:C:26:A:C6	1:C:27:U:C5	2.88	0.61
2:A:164:PRO:HG2	2:A:188:VAL:HG21	1.81	0.61
3:B:458:ASP:O	3:B:462:GLU:HG2	2.00	0.61
1:C:8:U:H5'	1:C:48:C:O2'	1.99	0.61
3:B:736:LEU:HD11	3:B:742:SER:HB2	1.83	0.61
3:B:285:THR:HG23	3:B:317:MET:SD	2.41	0.61
3:B:635:HIS:ND1	3:B:638:VAL:HG22	2.15	0.61
3:B:230:MET:O	3:B:234:LEU:HD22	2.00	0.61
2:A:54:LEU:HB3	2:A:58:LYS:NZ	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:85:ARG:HG3	2:A:85:ARG:NH1	2.12	0.61
2:A:134:PHE:HD1	2:A:134:PHE:O	1.84	0.61
3:B:548:LEU:HD13	3:B:576:VAL:HG23	1.83	0.60
1:C:24:G:H2'	1:C:25:C:O4'	2.00	0.60
3:B:283:LEU:HD23	3:B:284:LYS:N	2.16	0.60
3:B:149:ALA:C	3:B:151:PRO:HD3	2.25	0.60
2:A:32:LEU:CA	2:A:36:MET:HG2	2.31	0.60
2:A:101:HIS:NE2	2:A:103:ILE:HG13	2.17	0.60
2:A:307:TYR:CD1	2:A:307:TYR:N	2.66	0.60
2:A:120:GLN:HE21	3:B:489:GLU:HB2	1.66	0.60
2:A:260:PHE:HD1	2:A:261:VAL:HG13	1.66	0.60
3:B:17:SER:HB3	3:B:20:VAL:HB	1.83	0.60
2:A:54:LEU:HB3	2:A:58:LYS:HZ1	1.67	0.60
2:A:114:PHE:CZ	2:A:240:LEU:HG	2.36	0.60
2:A:165:LEU:HD23	2:A:165:LEU:H	1.66	0.60
2:A:48:ARG:O	2:A:52:GLN:HG3	2.00	0.59
2:A:329:ILE:HG23	2:A:330:PRO:HD2	1.82	0.59
2:A:258:PHE:HB2	2:A:261:VAL:HG22	1.83	0.59
1:C:18:G:N2	1:C:55:U:O2	2.28	0.59
2:A:29:LYS:O	2:A:33:THR:HG23	2.02	0.59
3:B:655:LEU:O	3:B:657:PRO:HD3	2.02	0.59
3:B:120:PRO:HG3	3:B:133:LEU:CD2	2.32	0.59
3:B:249:THR:HA	3:B:260:MET:HE2	1.84	0.59
1:C:10:G:N3	1:C:10:G:H2'	2.17	0.59
1:C:76:A:H5''	2:A:148:MET:HB3	1.85	0.59
2:A:182:MET:HG2	2:A:198:VAL:HG11	1.84	0.59
3:B:470:GLU:HA	3:B:470:GLU:OE1	2.02	0.59
2:A:46:GLU:O	2:A:50:ARG:HB3	2.02	0.59
3:B:651:PHE:CE2	3:B:672:GLU:HB3	2.38	0.59
2:A:250:LYS:H	2:A:270:TRP:HB3	1.68	0.59
3:B:666:PRO:HB2	3:B:667:PRO:HD2	1.84	0.59
1:C:33:U:H6	1:C:33:U:O5'	1.85	0.59
2:A:48:ARG:HB2	2:A:49:LYS:HD2	1.85	0.59
3:B:191:LEU:CD2	3:B:377:LEU:HB2	2.33	0.59
2:A:193:PRO:HB2	3:B:479:PHE:CE1	2.38	0.59
3:B:299:VAL:HG13	3:B:312:GLY:O	2.03	0.59
2:A:134:PHE:HB2	2:A:139:ILE:HB	1.84	0.58
1:C:25:C:H2'	1:C:26:A:O4'	2.03	0.58
1:C:31:A:H2'	1:C:32:C:C5'	2.33	0.58
1:C:29:C:H2'	1:C:30:G:H8	1.68	0.58
2:A:201:ARG:HD3	2:A:215:VAL:HG11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:455:LEU:HD12	3:B:455:LEU:N	2.18	0.58
3:B:589:LEU:HD21	3:B:608:LEU:HD23	1.85	0.58
2:A:133:ASN:HD21	2:A:178:HIS:CD2	2.22	0.58
3:B:259:PRO:HB3	3:B:356:ALA:HB1	1.85	0.58
2:A:103:ILE:O	2:A:107:GLU:HB2	2.03	0.58
3:B:454:ARG:HB2	3:B:455:LEU:HD12	1.85	0.58
1:C:49:C:H6	1:C:49:C:O5'	1.87	0.58
2:A:126:GLU:HG2	2:A:203:PHE:CE1	2.38	0.58
2:A:195:ARG:HG2	2:A:223:VAL:HG13	1.86	0.58
3:B:510:VAL:HG11	3:B:552:LEU:HD21	1.85	0.58
1:C:29:C:H2'	1:C:30:G:C8	2.39	0.58
2:A:150:ASP:HB3	2:A:205:PHE:HB3	1.84	0.58
3:B:698:ALA:HB3	3:B:780:ARG:HG2	1.85	0.58
3:B:747:LEU:HD23	3:B:749:PHE:CZ	2.39	0.57
3:B:590:PHE:CD1	3:B:591:GLY:N	2.73	0.57
1:C:15:G:H22	1:C:48:C:H42	1.52	0.57
3:B:546:THR:HG22	3:B:578:ARG:HB3	1.87	0.57
2:A:94:SER:HB3	3:B:567:ARG:HH12	1.68	0.57
3:B:673:LEU:HD23	3:B:673:LEU:N	2.20	0.57
2:A:238:TYR:HA	2:A:251:VAL:HG11	1.87	0.57
3:B:631:PHE:HB2	3:B:634:LEU:HD12	1.86	0.57
3:B:9:LYS:HA	3:B:12:VAL:O	2.05	0.57
3:B:695:ARG:CD	3:B:761:VAL:HG11	2.34	0.56
3:B:222:ARG:HH11	3:B:222:ARG:HG2	1.70	0.56
2:A:106:MET:HG2	2:A:323:ALA:HB2	1.86	0.56
2:A:143:HIS:C	2:A:145:ALA:H	2.13	0.56
3:B:638:VAL:HG23	3:B:638:VAL:O	2.05	0.56
1:C:45:U:C2	1:C:46:G:H5''	2.41	0.56
2:A:85:ARG:HH11	2:A:85:ARG:CG	2.17	0.56
2:A:50:ARG:O	2:A:54:LEU:HD22	2.06	0.56
2:A:306:ALA:HB3	2:A:307:TYR:CE1	2.40	0.56
3:B:42:PRO:HG2	3:B:96:LEU:HD23	1.88	0.56
3:B:90:ALA:HB2	3:B:118:LEU:HD21	1.87	0.56
3:B:99:LEU:CD2	3:B:101:GLN:HB3	2.35	0.56
3:B:353:ARG:HD3	3:B:353:ARG:H	1.69	0.56
1:C:9:A:N6	1:C:22:G:C6	2.74	0.55
3:B:33:ASP:HB2	3:B:157:ASP:HB3	1.86	0.55
3:B:298:LEU:O	3:B:313:LEU:HD23	2.06	0.55
1:C:27:U:H2'	1:C:28:G:C8	2.39	0.55
3:B:423:GLU:O	3:B:427:ILE:HG12	2.06	0.55
3:B:695:ARG:HD3	3:B:761:VAL:HG11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:15:LEU:HD12	2:A:18:LEU:HD12	1.87	0.55
2:A:19:LYS:HG3	2:A:68:ARG:CG	2.36	0.55
2:A:165:LEU:CD1	2:A:303:LEU:HD11	2.36	0.55
2:A:186:TYR:CZ	2:A:190:HIS:ND1	2.73	0.55
3:B:128:TYR:CG	3:B:240:ARG:HD2	2.41	0.55
2:A:27:GLY:O	2:A:31:LEU:HD12	2.06	0.55
3:B:210:ALA:N	3:B:211:PRO:HD3	2.20	0.55
3:B:573:VAL:O	3:B:573:VAL:HG12	2.06	0.55
3:B:141:PRO:HB2	3:B:144:THR:HG23	1.88	0.55
3:B:12:VAL:HG22	3:B:15:LEU:CD1	2.30	0.55
1:C:45:U:C3'	1:C:46:G:C5'	2.84	0.55
3:B:250:ASN:O	3:B:254:LEU:HG	2.07	0.55
3:B:469:TYR:HA	3:B:472:ILE:CD1	2.37	0.55
1:C:68:U:O5'	1:C:68:U:H6	1.90	0.55
2:A:28:LYS:O	2:A:32:LEU:N	2.40	0.55
2:A:223:VAL:HB	2:A:313:PHE:CZ	2.41	0.55
2:A:263:PRO:HG3	3:B:461:GLU:HB2	1.88	0.55
2:A:42:LEU:H	2:A:43:PRO:CD	2.18	0.55
2:A:327:TYR:N	2:A:327:TYR:HD2	2.05	0.55
1:C:61:C:C5	1:C:62:C:H5	2.25	0.54
1:C:68:U:C6	1:C:68:U:H3'	2.43	0.54
2:A:108:ARG:O	2:A:112:GLU:HG3	2.07	0.54
3:B:276:ARG:HH11	3:B:276:ARG:HG3	1.71	0.54
3:B:463:VAL:O	3:B:467:GLN:HB2	2.06	0.54
3:B:604:SER:HA	3:B:608:LEU:HB2	1.89	0.54
2:A:49:LYS:HD2	2:A:49:LYS:N	2.20	0.54
3:B:290:GLU:HG3	3:B:290:GLU:O	2.06	0.54
1:C:33:U:O2'	1:C:35:A:N7	2.24	0.54
1:C:47:U:C3'	1:C:48:C:C5'	2.83	0.54
3:B:267:PHE:N	3:B:267:PHE:CD1	2.76	0.54
2:A:134:PHE:O	2:A:135:ASP:HB2	2.07	0.54
3:B:594:VAL:HG12	3:B:595:GLY:N	2.22	0.54
1:C:45:U:H3'	1:C:46:G:H5'	1.88	0.54
2:A:287:HIS:HD2	2:A:288:PRO:CD	2.20	0.54
2:A:86:VAL:HG12	2:A:87:ASP:N	2.21	0.54
2:A:262:GLU:OE2	3:B:458:ASP:HA	2.08	0.54
1:C:32:C:H2'	1:C:33:U:H5'	1.89	0.54
2:A:162:GLU:OE2	3:B:580:ARG:HD3	2.08	0.54
3:B:7:TRP:O	3:B:10:ALA:HB3	2.07	0.54
3:B:589:LEU:HD23	3:B:609:LEU:HB2	1.89	0.54
3:B:593:GLY:HA3	3:B:604:SER:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:656:HIS:CD2	3:B:658:GLU:HG3	2.43	0.54
3:B:189:ALA:HB1	3:B:378:SER:CB	2.38	0.53
3:B:706:PRO:CG	3:B:709:GLU:HB2	2.21	0.53
2:A:50:ARG:HA	2:A:54:LEU:HD13	1.89	0.53
3:B:44:GLY:HA3	3:B:94:THR:OG1	2.07	0.53
2:A:184:VAL:HG22	2:A:294:VAL:HG12	1.91	0.53
2:A:195:ARG:HG2	2:A:223:VAL:CG2	2.38	0.53
3:B:84:GLY:O	3:B:137:GLU:HB3	2.08	0.53
3:B:701:VAL:CG2	3:B:705:THR:HG21	2.38	0.53
3:B:731:TYR:O	3:B:741:LYS:HA	2.09	0.53
2:A:9:ILE:O	2:A:13:ARG:HG2	2.07	0.53
3:B:772:LEU:HD12	3:B:779:LEU:HD21	1.91	0.53
2:A:120:GLN:NE2	3:B:489:GLU:HB2	2.23	0.53
3:B:156:LEU:HD23	3:B:156:LEU:N	2.24	0.53
3:B:294:HIS:CD2	3:B:296:GLU:HB2	2.41	0.53
3:B:701:VAL:HG12	3:B:777:PHE:CD2	2.44	0.53
3:B:120:PRO:CA	3:B:133:LEU:HD21	2.39	0.52
2:A:165:LEU:HD23	2:A:165:LEU:N	2.25	0.52
3:B:491:PRO:O	3:B:494:LYS:HG2	2.08	0.52
1:C:55:U:O4	1:C:57:G:OP2	2.26	0.52
2:A:165:LEU:HD13	2:A:303:LEU:HD11	1.92	0.52
3:B:390:GLU:O	3:B:391:ALA:HB2	2.08	0.52
3:B:498:LEU:HG	3:B:502:LEU:HD23	1.90	0.52
2:A:202:VAL:HG21	2:A:218:GLN:HG3	1.90	0.52
1:C:9:A:N3	1:C:45:U:O4	2.43	0.52
3:B:300:ILE:HG12	3:B:314:ALA:HB2	1.90	0.52
3:B:665:LEU:HB2	3:B:666:PRO:HD2	1.92	0.52
1:C:63:G:H2'	1:C:64:C:H6	1.69	0.52
2:A:49:LYS:O	2:A:54:LEU:HD13	2.10	0.52
3:B:120:PRO:HA	3:B:133:LEU:HD21	1.91	0.52
3:B:39:PHE:H	3:B:40:PRO:HD3	1.75	0.52
3:B:404:ILE:HG22	3:B:405:PRO:HD2	1.91	0.52
1:C:61:C:H3'	1:C:61:C:H6	1.74	0.52
3:B:115:GLY:O	3:B:116:MET:HB3	2.09	0.52
3:B:200:PHE:HE1	3:B:215:LEU:HB3	1.75	0.52
3:B:566:GLU:O	3:B:591:GLY:HA3	2.09	0.52
1:C:35:A:N1	1:C:36:A:C5	2.78	0.51
2:A:32:LEU:C	2:A:36:MET:HG2	2.35	0.51
3:B:245:VAL:HG11	3:B:324:VAL:HG11	1.91	0.51
3:B:232:ARG:O	3:B:236:ALA:HB2	2.11	0.51
3:B:301:ALA:HB1	3:B:309:PHE:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:A:H8	2:A:149:TRP:CE2	2.27	0.51
3:B:517:ASP:HB3	3:B:540:GLU:O	2.09	0.51
1:C:43:A:O2'	1:C:44:G:H5'	2.11	0.51
1:C:50:G:H2'	1:C:51:C:O4'	2.10	0.51
2:A:88:VAL:HG23	2:A:89:SER:N	2.26	0.51
3:B:672:GLU:C	3:B:673:LEU:HD23	2.36	0.51
2:A:106:MET:HG3	2:A:319:VAL:HG13	1.93	0.51
2:A:140:PRO:HD2	2:A:143:HIS:HD2	1.75	0.51
2:A:165:LEU:HD21	2:A:301:LEU:HD13	1.93	0.51
2:A:181:PRO:O	2:A:184:VAL:HG12	2.10	0.51
3:B:3:VAL:HG23	3:B:156:LEU:O	2.10	0.51
3:B:193:ALA:HB3	3:B:390:GLU:HB2	1.92	0.51
2:A:336:PHE:HB3	3:B:513:TYR:CE1	2.46	0.51
3:B:1:MET:CG	3:B:2:ARG:H	2.22	0.51
3:B:121:ARG:HG3	3:B:121:ARG:HH11	1.76	0.51
2:A:13:ARG:HE	2:A:72:LEU:HD22	1.75	0.51
2:A:245:PHE:HE1	2:A:269:VAL:HG21	1.76	0.50
3:B:214:THR:HB	3:B:335:VAL:O	2.11	0.50
3:B:403:ALA:HA	3:B:444:VAL:O	2.12	0.50
3:B:764:ALA:HA	3:B:767:ARG:NH1	2.27	0.50
1:C:1:G:O5'	1:C:1:G:H8	1.95	0.50
3:B:698:ALA:HB3	3:B:780:ARG:HG3	1.91	0.50
3:B:16:GLU:O	3:B:17:SER:CB	2.59	0.50
3:B:39:PHE:HB2	3:B:152:GLU:HA	1.92	0.50
3:B:50:VAL:HA	3:B:66:LEU:HD23	1.92	0.50
1:C:16:U:O2'	1:C:17:U:C6	2.65	0.50
1:C:20:U:O2'	1:C:21:A:OP1	2.23	0.50
2:A:196:ILE:HD11	2:A:222:LEU:HD21	1.94	0.50
2:A:119:TYR:OH	2:A:223:VAL:HG21	2.11	0.50
2:A:201:ARG:HD3	2:A:215:VAL:CG1	2.42	0.50
3:B:213:PHE:CE2	3:B:215:LEU:HD13	2.43	0.50
3:B:502:LEU:O	3:B:507:PHE:HB2	2.11	0.50
3:B:510:VAL:CG1	3:B:552:LEU:HD21	2.41	0.50
3:B:556:LEU:O	3:B:556:LEU:HG	2.10	0.50
2:A:149:TRP:CD1	2:A:204:ARG:NH1	2.80	0.50
1:C:31:A:C2'	1:C:32:C:C5'	2.88	0.50
2:A:131:PHE:O	2:A:135:ASP:HB3	2.11	0.50
2:A:196:ILE:HD11	2:A:222:LEU:CD2	2.42	0.50
3:B:610:LYS:O	3:B:614:GLU:HG2	2.11	0.50
3:B:674:ARG:HB3	3:B:674:ARG:NH1	2.26	0.50
1:C:76:A:C8	2:A:149:TRP:CE2	3.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:230:MET:HE2	3:B:415:LEU:CD2	2.41	0.50
3:B:60:ARG:HH22	3:B:79:GLU:HG3	1.76	0.50
3:B:284:LYS:HA	3:B:289:VAL:O	2.12	0.50
3:B:607:PHE:HA	3:B:610:LYS:HB3	1.94	0.50
1:C:38:A:H2'	1:C:39:U:H5'	1.94	0.49
2:A:164:PRO:HD2	2:A:167:GLU:OE2	2.12	0.49
3:B:324:VAL:HG13	3:B:328:THR:HG21	1.94	0.49
3:B:496:GLN:HE21	3:B:496:GLN:HA	1.78	0.49
3:B:551:GLY:O	3:B:555:VAL:HB	2.12	0.49
3:B:715:ARG:HB3	3:B:715:ARG:HH11	1.77	0.49
3:B:285:THR:O	3:B:285:THR:HG22	2.11	0.49
3:B:656:HIS:O	3:B:659:ILE:HG13	2.12	0.49
3:B:692:ALA:HB1	3:B:749:PHE:O	2.13	0.49
3:B:722:LEU:HG	3:B:723:GLU:N	2.26	0.49
2:A:128:GLU:CG	2:A:129:SER:H	2.25	0.49
2:A:340:LEU:HB2	3:B:559:ASN:OD1	2.12	0.49
3:B:226:SER:HB3	3:B:244:ASN:HA	1.92	0.49
3:B:578:ARG:O	3:B:579:GLU:HB2	2.13	0.49
1:C:8:U:H4'	1:C:48:C:C1'	2.29	0.49
3:B:14:GLU:O	3:B:14:GLU:CG	2.60	0.49
2:A:233:LEU:HD13	2:A:313:PHE:HD1	1.76	0.49
3:B:364:VAL:O	3:B:366:PRO:HD3	2.13	0.49
3:B:12:VAL:CG2	3:B:15:LEU:HD13	2.31	0.49
3:B:242:ILE:HB	3:B:246:VAL:HG11	1.94	0.49
1:C:36:A:C6	1:C:37:A:N7	2.81	0.49
3:B:456:GLU:O	3:B:459:LEU:HB2	2.13	0.49
3:B:617:PHE:O	3:B:620:LEU:HB2	2.11	0.49
3:B:680:LYS:HE2	3:B:680:LYS:HB3	1.65	0.49
2:A:12:ALA:O	2:A:72:LEU:HD11	2.13	0.49
2:A:143:HIS:C	2:A:145:ALA:N	2.71	0.49
3:B:304:ARG:O	3:B:306:GLU:N	2.46	0.49
1:C:48:C:C2'	1:C:49:C:OP2	2.60	0.49
2:A:190:HIS:HB3	3:B:485:ASN:ND2	2.28	0.49
2:A:32:LEU:HA	2:A:36:MET:CG	2.41	0.48
2:A:134:PHE:HB3	2:A:139:ILE:HD12	1.95	0.48
3:B:102:LYS:HG2	3:B:103:VAL:O	2.13	0.48
3:B:572:GLU:HG3	3:B:573:VAL:N	2.28	0.48
3:B:666:PRO:CB	3:B:667:PRO:HD2	2.43	0.48
2:A:287:HIS:CD2	2:A:288:PRO:CD	2.91	0.48
3:B:198:LEU:HD21	3:B:391:ALA:HB3	1.96	0.48
3:B:498:LEU:O	3:B:502:LEU:HD23	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:700:VAL:HG22	3:B:778:GLY:O	2.12	0.48
1:C:8:U:O4	1:C:14:A:OP2	2.32	0.48
3:B:17:SER:CB	3:B:20:VAL:HB	2.44	0.48
2:A:130:GLU:O	2:A:135:ASP:HB2	2.14	0.48
3:B:478:ALA:O	3:B:479:PHE:HB3	2.14	0.48
3:B:545:ARG:NH1	3:B:548:LEU:HD12	2.28	0.48
3:B:609:LEU:CD1	3:B:652:LEU:CD1	2.88	0.48
2:A:297:TYR:CD1	2:A:301:LEU:HD11	2.49	0.48
3:B:530:ARG:HG2	3:B:579:GLU:H	1.79	0.48
3:B:222:ARG:HH11	3:B:222:ARG:HG3	1.77	0.48
3:B:780:ARG:HD3	3:B:785:PRO:CG	2.43	0.48
2:A:12:ALA:C	2:A:72:LEU:HD11	2.38	0.48
2:A:32:LEU:HD22	2:A:36:MET:HE2	1.96	0.48
3:B:355:GLU:HG3	3:B:359:ARG:NH1	2.29	0.48
3:B:469:TYR:HA	3:B:472:ILE:HD12	1.95	0.48
3:B:556:LEU:HD23	3:B:665:LEU:HD22	1.96	0.48
3:B:564:ARG:N	3:B:565:PRO:HD3	2.29	0.48
3:B:576:VAL:HG11	3:B:584:HIS:CD2	2.48	0.48
2:A:143:HIS:CD2	2:A:145:ALA:HB3	2.49	0.47
3:B:149:ALA:O	3:B:151:PRO:HD3	2.14	0.47
3:B:282:ARG:HG2	3:B:292:THR:HA	1.96	0.47
3:B:592:GLU:HB2	3:B:602:ARG:HG3	1.95	0.47
2:A:91:PRO:HB2	3:B:597:PRO:CG	2.41	0.47
3:B:166:ASP:O	3:B:172:GLY:HA3	2.13	0.47
3:B:192:LYS:HD3	3:B:192:LYS:N	2.29	0.47
3:B:209:GLY:HA3	3:B:298:LEU:HD11	1.96	0.47
3:B:285:THR:HB	3:B:289:VAL:HG23	1.96	0.47
3:B:67:ASP:C	3:B:69:GLY:H	2.22	0.47
1:C:74:C:H42	1:C:75:C:H5	1.61	0.47
2:A:140:PRO:HD2	2:A:143:HIS:CD2	2.49	0.47
2:A:152:PHE:CE1	2:A:204:ARG:O	2.68	0.47
2:A:234:LYS:HE2	3:B:474:LEU:CD2	2.44	0.47
3:B:102:LYS:HE3	3:B:102:LYS:HB3	1.53	0.47
3:B:215:LEU:CD2	3:B:272:ILE:HG13	2.42	0.47
3:B:674:ARG:HB3	3:B:674:ARG:CZ	2.44	0.47
2:A:72:LEU:HD23	2:A:72:LEU:O	2.15	0.47
2:A:195:ARG:HG2	2:A:223:VAL:CG1	2.43	0.47
3:B:39:PHE:N	3:B:40:PRO:CD	2.75	0.47
3:B:60:ARG:HD2	3:B:60:ARG:O	2.14	0.47
3:B:507:PHE:CD2	3:B:569:LEU:HG	2.50	0.47
2:A:271:TRP:O	2:A:272:PRO:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:556:LEU:CD2	3:B:665:LEU:HD22	2.44	0.47
3:B:695:ARG:HD3	3:B:761:VAL:CG1	2.45	0.47
1:C:41:G:H2'	1:C:42:C:H5'	1.96	0.47
1:C:68:U:O2'	1:C:69:C:H5'	2.13	0.47
1:C:69:C:H2'	1:C:70:G:H8	1.79	0.47
2:A:16:GLU:HB3	2:A:72:LEU:HD12	1.96	0.47
2:A:143:HIS:CE1	2:A:145:ALA:HB2	2.50	0.47
3:B:193:ALA:HB2	3:B:388:VAL:HG23	1.97	0.47
3:B:286:LEU:HD23	3:B:317:MET:CE	2.41	0.47
3:B:722:LEU:HD21	3:B:725:LEU:HB2	1.95	0.47
2:A:122:VAL:O	2:A:198:VAL:HG13	2.15	0.47
3:B:145:PRO:HB2	3:B:148:GLU:HG2	1.97	0.47
3:B:566:GLU:HB3	3:B:592:GLU:OE1	2.15	0.47
3:B:699:VAL:HG13	3:B:772:LEU:HD13	1.97	0.47
2:A:192:PRO:O	3:B:482:ALA:HB2	2.15	0.47
3:B:257:ALA:O	3:B:259:PRO:HD3	2.15	0.47
3:B:415:LEU:O	3:B:472:ILE:HG23	2.15	0.47
3:B:613:LEU:O	3:B:616:LEU:HB3	2.14	0.47
2:A:97:SER:HB3	2:A:347:LYS:NZ	2.30	0.47
2:A:102:PRO:HA	2:A:105:LEU:CD1	2.43	0.47
2:A:234:LYS:HB3	3:B:474:LEU:CD2	2.43	0.47
3:B:644:VAL:O	3:B:645:GLU:C	2.58	0.47
1:C:27:U:H5'	3:B:564:ARG:NH2	2.30	0.46
1:C:71:G:H3'	1:C:71:G:C8	2.50	0.46
3:B:75:VAL:HG22	3:B:108:ILE:HD12	1.96	0.46
3:B:518:PRO:HD3	3:B:542:ALA:HB3	1.97	0.46
1:C:21:A:C2	1:C:48:C:C5	3.04	0.46
2:A:132:PHE:HE1	2:A:164:PRO:HD3	1.80	0.46
2:A:263:PRO:CB	3:B:461:GLU:HB2	2.45	0.46
3:B:641:ARG:HA	3:B:651:PHE:HA	1.97	0.46
2:A:229:ALA:O	2:A:232:HIS:HB2	2.15	0.46
2:A:235:GLY:O	2:A:238:TYR:HB3	2.16	0.46
3:B:255:GLU:OE1	3:B:375:ARG:NH1	2.48	0.46
2:A:240:LEU:HD11	2:A:317:LEU:HD11	1.98	0.46
3:B:193:ALA:HB1	3:B:390:GLU:N	2.31	0.46
3:B:699:VAL:O	3:B:742:SER:HA	2.16	0.46
3:B:736:LEU:O	3:B:738:GLU:N	2.46	0.46
3:B:252:VAL:HG12	3:B:252:VAL:O	2.15	0.46
3:B:509:GLU:HB2	3:B:571:PHE:HE2	1.81	0.46
3:B:589:LEU:HD12	3:B:590:PHE:H	1.81	0.46
1:C:76:A:H8	2:A:149:TRP:CZ2	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:585:LEU:HB2	3:B:675:LEU:HD11	1.96	0.46
1:C:47:U:O2	1:C:50:G:H5''	2.16	0.46
2:A:148:MET:HE3	3:B:162:PRO:HG2	1.98	0.46
2:A:148:MET:HB2	2:A:149:TRP:CE3	2.51	0.46
2:A:263:PRO:HB3	3:B:461:GLU:HB2	1.96	0.46
3:B:341:VAL:HA	3:B:344:ARG:HB3	1.97	0.46
2:A:142:HIS:CE1	3:B:345:LYS:HD2	2.51	0.46
3:B:496:GLN:HE21	3:B:496:GLN:CA	2.29	0.46
3:B:773:ARG:HH21	3:B:782:LEU:CD1	2.28	0.46
1:C:35:A:C2	1:C:36:A:C8	3.04	0.46
2:A:269:VAL:O	2:A:269:VAL:HG23	2.15	0.46
3:B:35:ILE:HD11	3:B:156:LEU:HD13	1.97	0.46
3:B:275:ARG:HG2	3:B:275:ARG:HH11	1.81	0.46
3:B:485:ASN:O	3:B:488:VAL:HG22	2.16	0.46
1:C:68:U:C6	1:C:68:U:C3'	2.99	0.45
2:A:141:GLU:HG2	2:A:146:ARG:CZ	2.45	0.45
2:A:195:ARG:CG	2:A:223:VAL:HG13	2.45	0.45
3:B:780:ARG:HD3	3:B:785:PRO:HG2	1.97	0.45
3:B:243:ASN:O	3:B:244:ASN:C	2.58	0.45
3:B:345:LYS:HA	3:B:345:LYS:HE2	1.99	0.45
1:C:55:U:H6	1:C:55:U:O5'	2.00	0.45
1:C:75:C:H2'	1:C:75:C:O2	2.16	0.45
2:A:53:GLU:HA	2:A:57:ILE:HD12	1.99	0.45
2:A:110:LEU:HD11	2:A:322:LEU:HD12	1.99	0.45
3:B:46:VAL:CG2	3:B:47:PHE:N	2.78	0.45
2:A:92:GLY:O	2:A:93:ALA:C	2.60	0.45
2:A:344:GLU:O	2:A:347:LYS:HG2	2.15	0.45
3:B:329:GLU:CD	3:B:329:GLU:N	2.75	0.45
1:C:24:G:O6	1:C:25:C:N3	2.50	0.45
1:C:58:A:C4'	1:C:59:U:OP1	2.33	0.45
2:A:271:TRP:CE3	2:A:274:GLY:HA3	2.52	0.45
3:B:242:ILE:HB	3:B:246:VAL:CG1	2.47	0.45
3:B:631:PHE:CZ	3:B:641:ARG:HB3	2.52	0.45
3:B:751:HIS:HD2	3:B:753:LYS:HB3	1.80	0.45
1:C:27:U:C2	1:C:28:G:N7	2.85	0.45
3:B:1:MET:HG2	3:B:2:ARG:H	1.81	0.45
2:A:298:ARG:HH12	2:A:306:ALA:HB2	1.82	0.45
3:B:82:ARG:HG3	3:B:83:LYS:O	2.17	0.45
3:B:173:LEU:HA	3:B:173:LEU:HD13	1.66	0.45
3:B:707:TYR:O	3:B:709:GLU:N	2.50	0.45
3:B:780:ARG:CD	3:B:785:PRO:HG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:132:PHE:HD2	2:A:132:PHE:HA	1.63	0.45
2:A:180:SER:N	2:A:181:PRO:HD2	2.32	0.45
3:B:430:ARG:HH11	3:B:430:ARG:CB	2.30	0.45
3:B:430:ARG:NH1	3:B:430:ARG:HB3	2.32	0.45
3:B:459:LEU:O	3:B:462:GLU:HB2	2.16	0.45
3:B:697:LEU:C	3:B:697:LEU:HD12	2.42	0.45
1:C:47:U:H5'	1:C:48:C:OP2	2.17	0.44
2:A:240:LEU:O	2:A:244:LEU:HB2	2.17	0.44
3:B:202:LEU:HB2	3:B:215:LEU:HD23	2.00	0.44
3:B:464:ALA:O	3:B:469:TYR:CE2	2.70	0.44
3:B:512:THR:HG22	3:B:555:VAL:HG21	1.99	0.44
3:B:604:SER:CA	3:B:608:LEU:HD22	2.43	0.44
1:C:14:A:H2'	1:C:15:G:C5'	2.44	0.44
2:A:12:ALA:O	2:A:16:GLU:N	2.50	0.44
2:A:233:LEU:CD1	2:A:313:PHE:CD1	3.00	0.44
3:B:28:LEU:HD23	3:B:28:LEU:HA	1.68	0.44
2:A:132:PHE:C	2:A:133:ASN:O	2.59	0.44
2:A:208:THR:O	2:A:208:THR:HG22	2.16	0.44
2:A:213:GLU:HG3	2:A:332:ILE:HG23	1.99	0.44
2:A:263:PRO:CG	3:B:461:GLU:HB2	2.47	0.44
3:B:628:ALA:O	3:B:629:GLN:HB2	2.17	0.44
1:C:10:G:C2	1:C:11:C:C5	3.05	0.44
2:A:324:MET:O	2:A:328:GLY:HA2	2.17	0.44
3:B:56:ILE:HD11	3:B:63:ARG:HB2	1.99	0.44
1:C:24:G:N7	1:C:25:C:C6	2.86	0.44
1:C:27:U:C2	1:C:28:G:C8	3.06	0.44
3:B:25:LEU:HD13	3:B:158:LEU:HD21	2.00	0.44
3:B:213:PHE:HE2	3:B:215:LEU:CD1	2.28	0.44
2:A:28:LYS:O	2:A:32:LEU:HG	2.17	0.44
2:A:52:GLN:O	2:A:56:ALA:HB3	2.17	0.44
2:A:78:LYS:HA	2:A:81:LEU:HD12	1.98	0.44
2:A:228:ILE:N	2:A:228:ILE:CD1	2.80	0.44
3:B:707:TYR:HE1	3:B:745:PHE:HZ	1.65	0.44
2:A:67:ALA:O	2:A:71:ALA:HB3	2.18	0.44
3:B:2:ARG:HG3	3:B:155:VAL:CG1	2.47	0.44
3:B:120:PRO:HG3	3:B:133:LEU:HD21	1.99	0.44
3:B:209:GLY:C	3:B:211:PRO:HD3	2.43	0.44
2:A:133:ASN:ND2	2:A:178:HIS:CD2	2.86	0.44
3:B:461:GLU:HG2	3:B:461:GLU:O	2.17	0.44
3:B:703:ALA:O	3:B:741:LYS:HD3	2.18	0.44
3:B:710:VAL:HG21	3:B:743:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:65:LEU:O	2:A:69:GLU:HB3	2.18	0.44
2:A:183:GLN:CG	2:A:222:LEU:HD22	2.39	0.44
3:B:430:ARG:CB	3:B:430:ARG:NH1	2.80	0.44
3:B:701:VAL:HB	3:B:777:PHE:CE2	2.53	0.44
3:B:761:VAL:O	3:B:764:ALA:HB3	2.18	0.44
3:B:616:LEU:C	3:B:616:LEU:HD23	2.43	0.43
3:B:666:PRO:HB2	3:B:667:PRO:CD	2.48	0.43
2:A:329:ILE:HG23	2:A:330:PRO:CD	2.48	0.43
3:B:644:VAL:HG23	3:B:649:VAL:CG2	2.48	0.43
2:A:283:ALA:CB	2:A:315:PHE:HA	2.48	0.43
3:B:128:TYR:CB	3:B:240:ARG:HD2	2.48	0.43
3:B:730:LEU:CD1	3:B:743:LEU:CD2	2.91	0.43
1:C:26:A:C5	1:C:27:U:C5	3.06	0.43
2:A:266:GLN:O	2:A:266:GLN:HG3	2.18	0.43
3:B:758:ASP:C	3:B:760:GLU:N	2.76	0.43
2:A:134:PHE:O	2:A:134:PHE:CD1	2.68	0.43
2:A:182:MET:CG	2:A:198:VAL:HG11	2.48	0.43
2:A:198:VAL:N	2:A:220:GLU:O	2.45	0.43
2:A:221:GLY:O	2:A:314:ALA:HA	2.18	0.43
2:A:224:VAL:HG13	2:A:312:GLY:HA3	2.00	0.43
2:A:242:GLN:HE22	2:A:247:PRO:HA	1.83	0.43
3:B:47:PHE:CZ	3:B:139:ALA:HB3	2.54	0.43
2:A:197:VAL:HB	2:A:219:LEU:HD11	2.00	0.43
3:B:773:ARG:C	3:B:775:ARG:H	2.27	0.43
2:A:340:LEU:O	2:A:344:GLU:HG3	2.18	0.43
3:B:357:SER:O	3:B:360:PHE:N	2.51	0.43
3:B:407:ARG:NH2	3:B:410:TYR:CG	2.87	0.43
3:B:555:VAL:HG12	3:B:556:LEU:N	2.34	0.43
3:B:677:LEU:HB3	3:B:678:PRO:HD2	2.01	0.43
3:B:140:LEU:O	3:B:141:PRO:C	2.60	0.43
3:B:164:ARG:HD2	3:B:164:ARG:HA	1.36	0.43
3:B:165:PRO:HG2	3:B:451:LEU:HD23	2.00	0.43
3:B:408:PRO:O	3:B:411:ALA:HB3	2.18	0.43
2:A:232:HIS:HD2	3:B:477:PRO:HB3	1.83	0.43
2:A:271:TRP:HB2	2:A:278:LEU:HD22	1.99	0.43
3:B:365:ASP:C	3:B:367:LEU:H	2.27	0.43
3:B:596:LEU:HB2	3:B:599:ALA:CB	2.48	0.43
3:B:707:TYR:HE1	3:B:745:PHE:CZ	2.36	0.43
2:A:230:MET:HE2	3:B:415:LEU:HD22	2.01	0.43
3:B:259:PRO:HB3	3:B:356:ALA:CB	2.48	0.43
3:B:260:MET:HB3	3:B:335:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:283:LEU:CD2	3:B:320:ALA:HB2	2.42	0.43
3:B:306:GLU:OE2	3:B:306:GLU:HA	2.19	0.43
3:B:531:LEU:HB2	3:B:544:LEU:HD12	2.00	0.43
2:A:16:GLU:HB3	2:A:72:LEU:CD1	2.49	0.42
2:A:128:GLU:HG2	2:A:181:PRO:HB3	2.00	0.42
2:A:195:ARG:HA	2:A:223:VAL:HG22	2.01	0.42
3:B:194:GLU:OE2	3:B:387:ARG:NH2	2.52	0.42
3:B:206:ASP:OD2	3:B:276:ARG:NH1	2.51	0.42
3:B:377:LEU:HB3	3:B:388:VAL:HG11	2.00	0.42
3:B:469:TYR:HA	3:B:472:ILE:HD11	2.01	0.42
3:B:573:VAL:HA	3:B:584:HIS:O	2.19	0.42
1:C:6:G:C2'	1:C:7:G:O5'	2.67	0.42
3:B:1:MET:N	3:B:158:LEU:O	2.52	0.42
3:B:520:ASP:O	3:B:521:ALA:C	2.62	0.42
2:A:140:PRO:O	2:A:143:HIS:HB2	2.19	0.42
1:C:8:U:O4	1:C:13:C:H2'	2.19	0.42
1:C:45:U:H2'	1:C:46:G:O5'	2.18	0.42
3:B:128:TYR:CD2	3:B:240:ARG:HD2	2.54	0.42
3:B:406:PHE:HA	3:B:456:GLU:HG3	2.02	0.42
3:B:430:ARG:HH11	3:B:430:ARG:HB2	1.83	0.42
2:A:105:LEU:HD13	2:A:349:VAL:HG21	2.02	0.42
3:B:99:LEU:HD23	3:B:101:GLN:HB3	1.99	0.42
3:B:80:ASN:O	3:B:82:ARG:NH1	2.52	0.42
3:B:223:VAL:HG13	3:B:243:ASN:HB2	2.01	0.42
3:B:507:PHE:CE2	3:B:569:LEU:HG	2.55	0.42
2:A:234:LYS:HB3	2:A:234:LYS:HE2	1.79	0.42
3:B:150:TRP:CZ2	3:B:232:ARG:HA	2.55	0.42
3:B:700:VAL:HG22	3:B:778:GLY:C	2.44	0.42
3:B:779:LEU:HB3	3:B:780:ARG:H	1.63	0.42
3:B:91:LEU:HD23	3:B:91:LEU:HA	1.89	0.42
3:B:309:PHE:HA	3:B:310:PRO:HD3	1.68	0.42
3:B:514:SER:O	3:B:545:ARG:HG2	2.20	0.42
2:A:220:GLU:HA	2:A:316:GLY:HA2	2.02	0.42
3:B:491:PRO:HG2	3:B:492:TYR:H	1.85	0.42
3:B:496:GLN:HA	3:B:496:GLN:NE2	2.35	0.42
3:B:734:PRO:CA	3:B:736:LEU:H	2.23	0.42
1:C:76:A:C8	2:A:149:TRP:NE1	2.88	0.42
2:A:110:LEU:HD12	2:A:319:VAL:HG22	2.02	0.42
2:A:178:HIS:CD2	2:A:178:HIS:H	2.38	0.42
3:B:467:GLN:HA	3:B:467:GLN:NE2	2.33	0.42
3:B:701:VAL:HA	3:B:702:PRO:HD2	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:C:O5'	1:C:49:C:C6	2.69	0.41
2:A:228:ILE:O	2:A:311:THR:HG21	2.19	0.41
3:B:265:LEU:HD23	3:B:265:LEU:HA	1.79	0.41
1:C:37:A:C6	1:C:38:A:C8	3.08	0.41
1:C:39:U:C2'	1:C:40:C:C5'	2.75	0.41
1:C:45:U:H2'	1:C:46:G:H5''	2.02	0.41
1:C:61:C:C4	1:C:62:C:C4	3.08	0.41
2:A:209:ASP:C	2:A:333:ARG:HE	2.27	0.41
2:A:303:LEU:O	2:A:304:PRO:C	2.63	0.41
3:B:21:LEU:O	3:B:24:ARG:N	2.53	0.41
3:B:96:LEU:HA	3:B:97:PRO:HD3	1.60	0.41
1:C:65:G:C2'	1:C:66:C:C5'	2.88	0.41
3:B:243:ASN:O	3:B:245:VAL:N	2.53	0.41
3:B:245:VAL:CG1	3:B:324:VAL:HG11	2.50	0.41
3:B:538:ALA:HB1	3:B:540:GLU:OE2	2.20	0.41
3:B:633:PHE:O	3:B:656:HIS:HB2	2.21	0.41
3:B:772:LEU:HB3	3:B:777:PHE:O	2.20	0.41
3:B:90:ALA:CB	3:B:118:LEU:HD21	2.50	0.41
3:B:364:VAL:HG12	3:B:365:ASP:N	2.35	0.41
3:B:715:ARG:CG	3:B:725:LEU:HD22	2.46	0.41
1:C:11:C:C2	1:C:12:U:C5	3.09	0.41
2:A:135:ASP:HB3	2:A:136:ALA:H	1.74	0.41
2:A:160:ARG:NE	3:B:580:ARG:HH21	2.19	0.41
3:B:614:GLU:HG2	3:B:614:GLU:H	1.65	0.41
3:B:728:PHE:CG	3:B:746:HIS:CD2	3.08	0.41
1:C:47:U:O5'	1:C:47:U:H6	2.04	0.41
2:A:49:LYS:H	2:A:49:LYS:CD	2.29	0.41
3:B:211:PRO:HD2	3:B:337:CYS:O	2.19	0.41
3:B:254:LEU:HD23	3:B:254:LEU:HA	1.77	0.41
3:B:692:ALA:HB2	3:B:750:ARG:HD2	2.03	0.41
2:A:132:PHE:CE1	2:A:164:PRO:HD3	2.55	0.41
1:C:36:A:N1	1:C:37:A:C8	2.88	0.41
2:A:23:ALA:O	2:A:27:GLY:N	2.51	0.41
3:B:153:GLU:HG3	3:B:154:VAL:N	2.35	0.41
3:B:171:LEU:HD21	3:B:186:GLU:HG3	2.03	0.41
3:B:243:ASN:H	3:B:246:VAL:HG12	1.85	0.41
1:C:26:A:N3	1:C:26:A:H2'	2.35	0.41
2:A:141:GLU:H	2:A:141:GLU:HG3	1.71	0.41
2:A:184:VAL:O	2:A:188:VAL:HG22	2.21	0.41
3:B:73:GLU:O	3:B:74:VAL:HG23	2.21	0.41
3:B:90:ALA:O	3:B:91:LEU:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:178:HIS:CD2	3:B:182:TYR:O	2.67	0.41
3:B:249:THR:HA	3:B:260:MET:HE3	2.00	0.41
3:B:289:VAL:HG21	3:B:291:ARG:CZ	2.51	0.41
3:B:420:PRO:HD2	3:B:423:GLU:OE2	2.21	0.41
3:B:482:ALA:HA	3:B:483:PRO:HD3	1.93	0.41
3:B:576:VAL:HG11	3:B:584:HIS:NE2	2.36	0.41
3:B:586:ALA:HA	3:B:671:PHE:O	2.20	0.41
3:B:594:VAL:CG1	3:B:595:GLY:N	2.83	0.41
1:C:61:C:C6	1:C:61:C:H3'	2.55	0.41
1:C:76:A:N7	2:A:149:TRP:HZ2	2.18	0.41
2:A:129:SER:O	2:A:130:GLU:C	2.64	0.41
2:A:298:ARG:NH1	2:A:306:ALA:HB2	2.36	0.41
3:B:370:VAL:O	3:B:373:GLN:HB2	2.21	0.41
3:B:404:ILE:HG21	3:B:455:LEU:C	2.46	0.41
1:C:9:A:N6	1:C:22:G:N7	2.68	0.40
2:A:50:ARG:HA	2:A:54:LEU:CD1	2.50	0.40
2:A:86:VAL:CG1	2:A:87:ASP:N	2.83	0.40
2:A:327:TYR:O	2:A:328:GLY:C	2.64	0.40
3:B:90:ALA:O	3:B:91:LEU:C	2.64	0.40
3:B:96:LEU:HB2	3:B:99:LEU:CD1	2.46	0.40
3:B:414:LEU:CD2	3:B:460:VAL:HG21	2.47	0.40
3:B:460:VAL:C	3:B:462:GLU:H	2.29	0.40
1:C:45:U:H2'	1:C:46:G:C5'	2.50	0.40
2:A:14:ASP:O	2:A:17:GLU:HB3	2.19	0.40
2:A:174:LEU:C	2:A:174:LEU:HD12	2.47	0.40
3:B:489:GLU:HG2	3:B:493:ARG:HG3	2.03	0.40
2:A:197:VAL:HB	2:A:219:LEU:CD1	2.51	0.40
3:B:353:ARG:H	3:B:353:ARG:CD	2.33	0.40
3:B:402:GLU:OE2	3:B:402:GLU:HA	2.21	0.40
3:B:589:LEU:O	3:B:590:PHE:CB	2.68	0.40
3:B:622:LEU:HA	3:B:645:GLU:OE1	2.21	0.40
2:A:27:GLY:O	2:A:31:LEU:HB2	2.22	0.40
3:B:455:LEU:N	3:B:455:LEU:CD1	2.84	0.40
3:B:499:ARG:O	3:B:503:SER:HB2	2.21	0.40
3:B:757:ARG:O	3:B:759:GLU:N	2.54	0.40
3:B:768:VAL:O	3:B:772:LEU:HG	2.22	0.40
1:C:67:C:C5	1:C:67:C:OP2	2.74	0.40
2:A:65:LEU:HD23	2:A:65:LEU:HA	1.89	0.40
2:A:126:GLU:OE2	3:B:575:ARG:HB2	2.22	0.40
2:A:138:ASN:C	2:A:138:ASN:HD22	2.30	0.40
2:A:139:ILE:HG12	2:A:259:PRO:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:56:ILE:HA	3:B:57:PRO:HD3	1.86	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	343/350 (98%)	286 (83%)	42 (12%)	15 (4%)	2	13
3	B	783/785 (100%)	647 (83%)	97 (12%)	39 (5%)	1	11
All	All	1126/1135 (99%)	933 (83%)	139 (12%)	54 (5%)	2	12

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	48	ARG
2	A	130	GLU
2	A	135	ASP
3	B	16	GLU
3	B	39	PHE
3	B	286	LEU
3	B	326	GLU
3	B	386	ALA
3	B	391	ALA
3	B	406	PHE
3	B	629	GLN
3	B	691	PRO
3	B	701	VAL
3	B	738	GLU
2	A	133	ASN
2	A	247	PRO
2	A	280	LEU

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Mol	Chain	Res	Type
2	A	320	GLU
2	A	328	GLY
2	A	338	GLY
3	B	97	PRO
3	B	139	ALA
3	B	244	ASN
3	B	305	GLY
3	B	725	LEU
3	B	757	ARG
2	A	272	PRO
3	B	17	SER
3	B	256	ARG
3	B	367	LEU
3	B	590	PHE
3	B	737	PRO
3	B	753	LYS
2	A	330	PRO
3	B	291	ARG
2	A	166	GLY
3	B	57	PRO
3	B	81	ALA
3	B	91	LEU
3	B	116	MET
3	B	127	GLU
3	B	319	GLY
3	B	421	GLU
3	B	748	ARG
3	B	758	ASP
3	B	784	THR
2	A	42	LEU
2	A	93	ALA
2	A	164	PRO
3	B	657	PRO
3	B	142	PRO
3	B	209	GLY
3	B	708	GLY
3	B	735	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	272/277 (98%)	223 (82%)	49 (18%)	2	8
3	B	630/630 (100%)	505 (80%)	125 (20%)	1	6
All	All	902/907 (99%)	728 (81%)	174 (19%)	1	6

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	24	ARG
2	A	25	TYR
2	A	34	GLN
2	A	36	MET
2	A	45	GLU
2	A	47	ARG
2	A	49	LYS
2	A	55	ASN
2	A	68	ARG
2	A	77	LEU
2	A	85	ARG
2	A	100	LEU
2	A	103	ILE
2	A	104	THR
2	A	120	GLN
2	A	122	VAL
2	A	126	GLU
2	A	132	PHE
2	A	134	PHE
2	A	135	ASP
2	A	151	THR
2	A	160	ARG
2	A	165	LEU
2	A	168	GLU
2	A	170	GLU
2	A	178	HIS
2	A	184	VAL
2	A	185	ARG
2	A	188	VAL
2	A	196	ILE
2	A	202	VAL

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Mol	Chain	Res	Type
2	A	206	GLU
2	A	213	GLU
2	A	219	LEU
2	A	224	VAL
2	A	228	ILE
2	A	240	LEU
2	A	256	VAL
2	A	278	LEU
2	A	301	LEU
2	A	310	VAL
2	A	311	THR
2	A	317	LEU
2	A	320	GLU
2	A	327	TYR
2	A	339	ARG
2	A	340	LEU
2	A	349	VAL
2	A	350	LEU
3	B	2	ARG
3	B	3	VAL
3	B	12	VAL
3	B	16	GLU
3	B	20	VAL
3	B	22	GLU
3	B	24	ARG
3	B	31	GLU
3	B	33	ASP
3	B	35	ILE
3	B	37	ARG
3	B	42	PRO
3	B	43	ARG
3	B	46	VAL
3	B	67	ASP
3	B	70	ARG
3	B	72	VAL
3	B	73	GLU
3	B	75	VAL
3	B	83	LYS
3	B	87	VAL
3	B	89	LEU
3	B	94	THR
3	B	106	ARG

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Mol	Chain	Res	Type
3	B	108	ILE
3	B	109	GLN
3	B	111	VAL
3	B	137	GLU
3	B	156	LEU
3	B	157	ASP
3	B	161	THR
3	B	170	LEU
3	B	173	LEU
3	B	176	ASP
3	B	184	LEU
3	B	198	LEU
3	B	203	LYS
3	B	215	LEU
3	B	222	ARG
3	B	226	SER
3	B	234	LEU
3	B	239	MET
3	B	242	ILE
3	B	260	MET
3	B	268	VAL
3	B	270	GLU
3	B	272	ILE
3	B	275	ARG
3	B	276	ARG
3	B	285	THR
3	B	289	VAL
3	B	296	GLU
3	B	298	LEU
3	B	307	GLU
3	B	313	LEU
3	B	317	MET
3	B	329	GLU
3	B	333	LEU
3	B	340	PRO
3	B	341	VAL
3	B	353	ARG
3	B	354	THR
3	B	361	GLU
3	B	362	ARG
3	B	374	ARG
3	B	375	ARG

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Mol	Chain	Res	Type
3	B	394	GLU
3	B	397	SER
3	B	399	LYS
3	B	404	ILE
3	B	409	GLU
3	B	434	ARG
3	B	438	GLU
3	B	441	THR
3	B	451	LEU
3	B	454	ARG
3	B	459	LEU
3	B	460	VAL
3	B	465	ARG
3	B	467	GLN
3	B	474	LEU
3	B	476	LEU
3	B	496	GLN
3	B	497	ARG
3	B	502	LEU
3	B	503	SER
3	B	505	LEU
3	B	508	GLN
3	B	519	GLU
3	B	526	LEU
3	B	529	PRO
3	B	530	ARG
3	B	532	LEU
3	B	540	GLU
3	B	544	LEU
3	B	548	LEU
3	B	550	PRO
3	B	555	VAL
3	B	556	LEU
3	B	557	LYS
3	B	570	LEU
3	B	576	VAL
3	B	577	PHE
3	B	583	THR
3	B	588	LEU
3	B	600	LYS
3	B	609	LEU
3	B	613	LEU

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Mol	Chain	Res	Type
3	B	614	GLU
3	B	626	VAL
3	B	641	ARG
3	B	655	LEU
3	B	659	ILE
3	B	670	LEU
3	B	673	LEU
3	B	679	ASP
3	B	680	LYS
3	B	701	VAL
3	B	711	GLU
3	B	715	ARG
3	B	716	GLU
3	B	738	GLU
3	B	754	ARG
3	B	763	GLU
3	B	775	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	34	GLN
2	A	55	ASN
2	A	120	GLN
2	A	133	ASN
2	A	138	ASN
2	A	142	HIS
2	A	143	HIS
2	A	178	HIS
2	A	207	GLN
2	A	232	HIS
2	A	287	HIS
3	B	178	HIS
3	B	258	GLN
3	B	294	HIS
3	B	350	HIS
3	B	358	HIS
3	B	373	GLN
3	B	381	GLN
3	B	467	GLN
3	B	485	ASN
3	B	496	GLN

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Mol	Chain	Res	Type
3	B	547	HIS
3	B	690	HIS
3	B	732	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	75/76 (98%)	33 (44%)	8 (10%)

All (33) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	2	C
1	C	7	G
1	C	8	U
1	C	10	G
1	C	11	C
1	C	12	U
1	C	17	U
1	C	18	G
1	C	20	U
1	C	21	A
1	C	22	G
1	C	33	U
1	C	35	A
1	C	40	C
1	C	46	G
1	C	47	U
1	C	48	C
1	C	49	C
1	C	50	G
1	C	51	C
1	C	54	U
1	C	56	C
1	C	57	G
1	C	58	A
1	C	59	U
1	C	60	U
1	C	61	C
1	C	67	C
1	C	69	C

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Mol	Chain	Res	Type
1	C	72	C
1	C	73	A
1	C	74	C
1	C	76	A

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	7	G
1	C	9	A
1	C	19	G
1	C	20	U
1	C	47	U
1	C	56	C
1	C	57	G
1	C	58	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	C	76/76 (100%)	3.43	67 (88%) 0 0	34, 49, 56, 58	76 (100%)
2	A	345/350 (98%)	0.64	49 (14%) 6 5	17, 55, 95, 138	71 (20%)
3	B	785/785 (100%)	0.26	19 (2%) 59 40	9, 62, 98, 140	0
All	All	1206/1211 (99%)	0.57	135 (11%) 10 9	9, 58, 98, 140	147 (12%)

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	76	A	8.2
2	A	8	ALA	6.4
1	C	63	G	6.4
2	A	26	LEU	6.0
2	A	39	LEU	5.9
1	C	56	C	5.2
2	A	35	GLU	5.2
1	C	4	G	5.2
1	C	19	G	5.1
1	C	73	A	5.1
2	A	21	LEU	5.1
1	C	70	G	5.1
1	C	18	G	4.8
2	A	9	ILE	4.8
2	A	10	GLN	4.7
1	C	57	G	4.6
1	C	48	C	4.6
1	C	10	G	4.6
2	A	65	LEU	4.6
1	C	51	C	4.5
3	B	784	THR	4.4
1	C	53	G	4.4
2	A	18	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	52	G	4.3
2	A	43	PRO	4.3
2	A	34	GLN	4.3
2	A	57	ILE	4.3
1	C	71	G	4.3
2	A	12	ALA	4.2
1	C	20	U	4.2
1	C	1	G	4.2
1	C	24	G	4.2
1	C	46	G	4.2
1	C	64	C	4.1
1	C	35	A	4.1
1	C	55	U	4.1
1	C	9	A	4.0
1	C	3	C	4.0
1	C	61	C	4.0
1	C	74	C	4.0
1	C	15	G	4.0
2	A	7	ALA	3.9
2	A	14	ASP	3.9
2	A	50	ARG	3.9
1	C	68	U	3.8
2	A	25	TYR	3.8
1	C	62	C	3.7
2	A	15	LEU	3.7
1	C	58	A	3.7
3	B	785	PRO	3.6
1	C	2	C	3.6
1	C	42	C	3.6
1	C	69	C	3.6
2	A	61	LEU	3.6
1	C	75	C	3.6
2	A	30	GLY	3.6
2	A	42	LEU	3.5
2	A	49	LYS	3.5
1	C	11	C	3.5
3	B	755	THR	3.4
1	C	5	A	3.4
1	C	32	C	3.3
1	C	7	G	3.3
1	C	34	G	3.3
1	C	36	A	3.3

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Mol	Chain	Res	Type	RSRZ
3	B	16	GLU	3.3
1	C	40	C	3.2
3	B	780	ARG	3.2
1	C	59	U	3.2
1	C	72	C	3.2
1	C	16	U	3.2
2	A	52	GLN	3.1
3	B	329	GLU	3.0
1	C	8	U	3.0
1	C	39	U	3.0
1	C	67	C	3.0
1	C	21	A	2.9
2	A	60	ALA	2.9
1	C	26	A	2.9
1	C	31	A	2.9
2	A	31	LEU	2.9
1	C	25	C	2.8
1	C	33	U	2.8
1	C	6	G	2.8
3	B	781	GLY	2.8
2	A	51	GLY	2.7
2	A	76	ALA	2.7
2	A	32	LEU	2.7
1	C	17	U	2.7
1	C	38	A	2.7
2	A	16	GLU	2.7
1	C	22	G	2.7
2	A	64	ALA	2.7
3	B	782	LEU	2.7
2	A	41	ALA	2.6
1	C	41	G	2.6
1	C	65	G	2.6
2	A	11	ASN	2.6
1	C	43	A	2.6
1	C	50	G	2.6
2	A	20	ALA	2.6
1	C	13	C	2.5
2	A	19	LYS	2.5
3	B	290	GLU	2.5
3	B	756	LEU	2.5
2	A	28	LYS	2.4
2	A	55	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	49	C	2.4
2	A	63	ALA	2.4
1	C	54	U	2.4
2	A	46	GLU	2.4
2	A	33	THR	2.3
1	C	37	A	2.3
2	A	22	LYS	2.3
3	B	279	GLU	2.3
1	C	47	U	2.3
3	B	783	ASP	2.3
2	A	44	LEU	2.2
3	B	204	VAL	2.2
2	A	56	ALA	2.2
2	A	158	GLY	2.2
1	C	23	A	2.2
3	B	294	HIS	2.2
2	A	23	ALA	2.2
1	C	66	C	2.1
3	B	690	HIS	2.1
2	A	59	ALA	2.1
3	B	739	GLY	2.1
2	A	142	HIS	2.1
2	A	17	GLU	2.1
2	A	79	GLU	2.1
3	B	54	HIS	2.0
3	B	98	GLY	2.0
3	B	99	LEU	2.0
2	A	144	PRO	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.