



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:56 AM UTC

PDB ID : 1J2B / pdb_00001j2b
Title : Crystal Structure Of Archaeosine tRNA-Guanine Transglycosylase Complexed With lambda-form tRNA(Val)
Authors : Ishitani, R.; Nureki, O.; Nameki, N.; Okada, N.; Nishimura, S.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2002-12-29
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

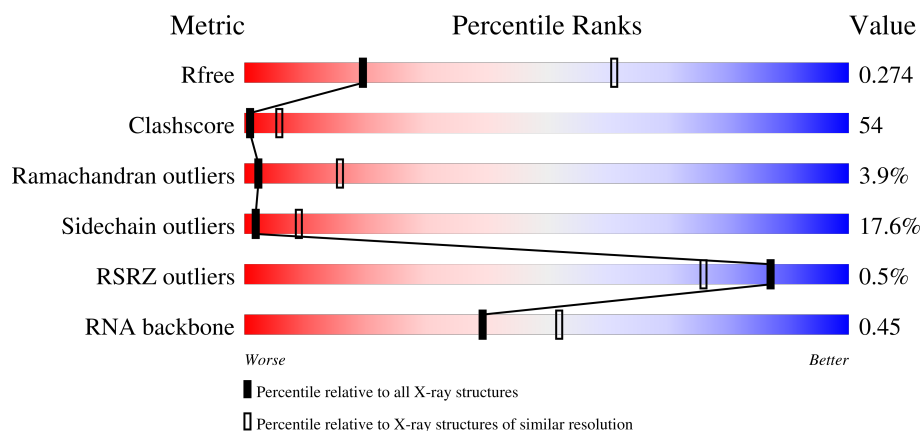
1 Overall quality at a glance

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	77	23% 47% 22% 8%
1	D	77	23% 43% 23% 8%
2	A	582	26% 57% 14% ..
2	B	582	25% 54% 19% ..

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12495 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(Val).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	77	Total	C	N	O	P	0	0	0
			1645	731	294	543	77			
1	D	71	Total	C	N	O	P	0	0	0
			1517	674	272	500	71			

- Molecule 2 is a protein called Archaeosine tRNA-guanine transglycosylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	576	Total	C	N	O	S	0	0	0
			4643	2964	813	847	19			
2	B	576	Total	C	N	O	S	0	0	0
			4643	2964	813	847	19			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	B	2	Total	Mg	0	0
			2	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		

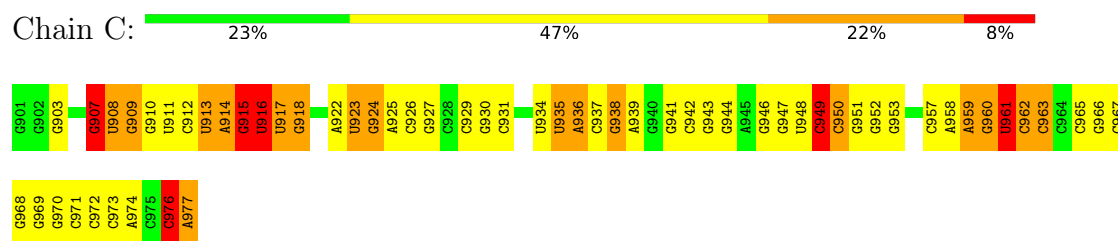
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	9	Total 9	O 9	0	0
5	D	8	Total 8	O 8	0	0
5	A	11	Total 11	O 11	0	0
5	B	13	Total 13	O 13	0	0

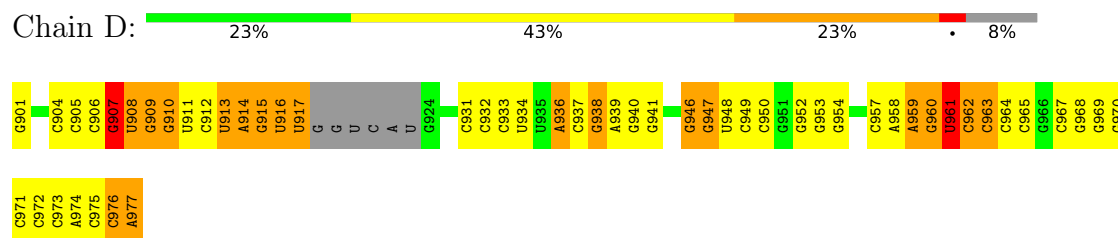
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

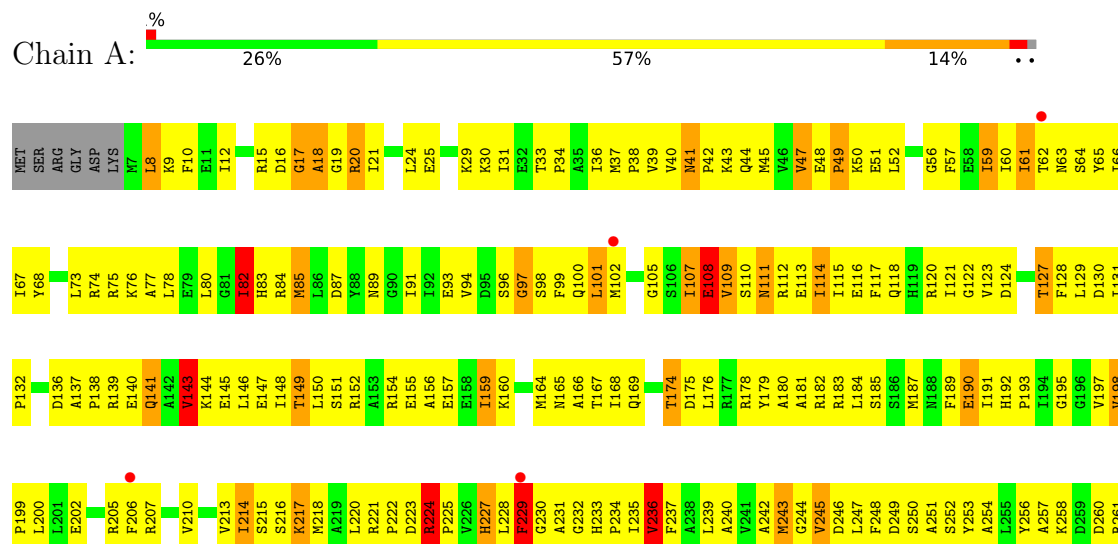
• Molecule 1: tRNA(Val)

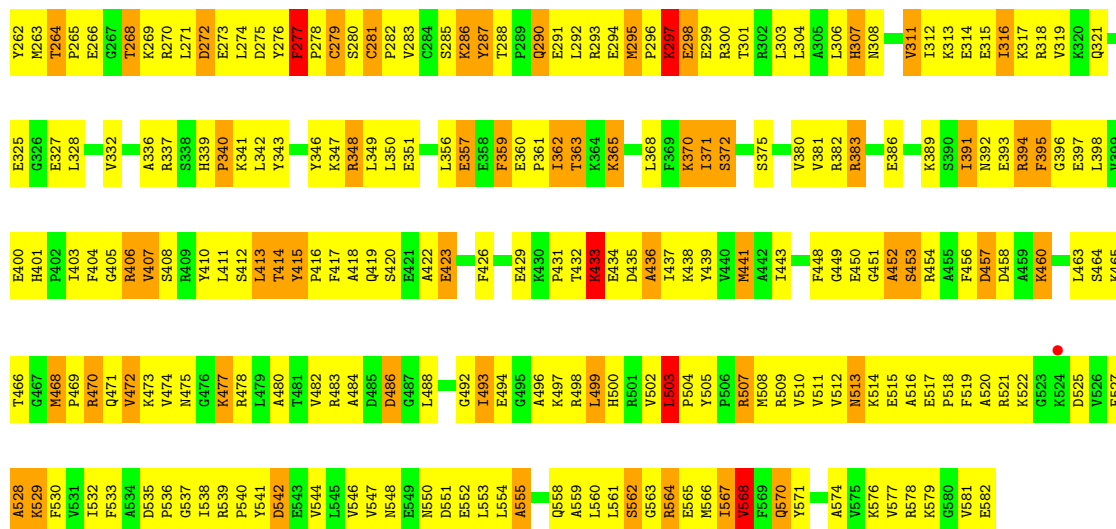


• Molecule 1: tRNA(Val)



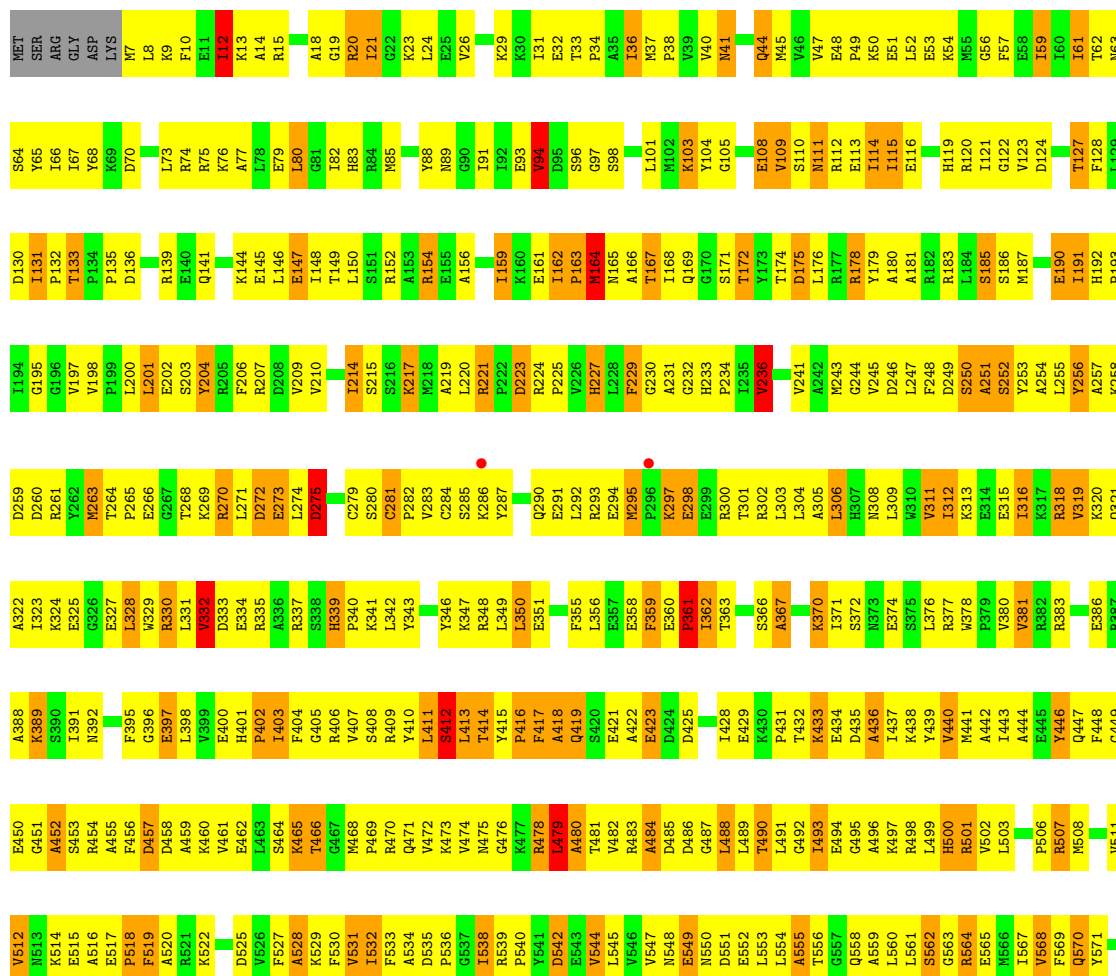
• Molecule 2: Archaeosine tRNA-guanine transglycosylase





● Molecule 2: Archaeosine tRNA-guanine transglycosylase

Chain B: 25% 54% 19% ..



V577		V581
R578		E582

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	230.83Å 230.83Å 269.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.54 – 3.30 48.54 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.54-3.30) 99.6 (48.54-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.19Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.225 , 0.288 0.221 , 0.274	Depositor DCC
R_{free} test set	4151 reflections (8.85%)	wwPDB-VP
Wilson B-factor (Å ²)	80.5	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 87.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.038 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.035 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.038 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12495	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	C	0.47	0/1836	0.90	8/2860 (0.3%)
1	D	0.44	0/1692	0.81	2/2633 (0.1%)
2	A	0.75	3/4736 (0.1%)	1.17	36/6380 (0.6%)
2	B	0.78	1/4736 (0.0%)	1.19	39/6380 (0.6%)
All	All	0.69	4/13000 (0.0%)	1.09	85/18253 (0.5%)

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	5
2	A	0	1
All	All	0	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	441	MET	SD-CE	5.97	1.94	1.79
2	A	508	MET	SD-CE	5.69	1.93	1.79
2	A	468	MET	SD-CE	5.35	1.93	1.79
2	B	12	ILE	CA-CB	5.24	1.58	1.53

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	223	ASP	N-CA-C	8.29	121.25	111.71
2	A	223	ASP	N-CA-C	8.16	122.33	112.38
2	B	41	ASN	CA-C-N	7.76	129.54	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	41	ASN	C-N-CA	7.76	129.54	119.84
1	C	961	U	N1-C1'-C2'	7.73	123.60	112.00
1	C	916	U	N1-C1'-C2'	7.61	123.41	112.00
2	B	544	VAL	N-CA-C	7.43	120.58	108.99
2	A	562	SER	N-CA-C	-7.23	100.96	110.43
1	D	907	G	C2'-C3'-O3'	7.21	120.31	109.50
2	B	275	ASP	N-CA-C	-7.00	104.86	113.41
2	B	367	ALA	N-CA-C	6.98	119.33	110.33
2	B	562	SER	N-CA-C	-6.98	101.32	110.53
2	B	484	ALA	N-CA-C	6.91	118.50	110.97
1	C	961	U	C4'-C3'-O3'	-6.75	102.87	113.00
2	A	97	GLY	N-CA-C	-6.72	105.47	114.95
2	A	275	ASP	N-CA-C	-6.66	105.45	113.97
2	A	236	VAL	CB-CA-C	-6.64	100.39	111.29
2	A	544	VAL	N-CA-C	6.64	119.92	108.95
2	B	97	GLY	N-CA-C	-6.46	105.84	114.95
2	B	91	ILE	CB-CA-C	-6.37	102.79	111.33
2	B	18	ALA	N-CA-C	-6.30	103.11	113.50
2	A	167	THR	N-CA-C	6.29	118.88	109.25
2	A	486	ASP	N-CA-C	6.12	120.06	112.59
2	B	251	ALA	N-CA-C	-5.95	106.00	113.20
2	B	319	VAL	CB-CA-C	-5.94	104.10	111.70
2	A	108	GLU	N-CA-C	5.92	117.93	108.41
2	B	263	MET	N-CA-C	5.90	118.85	109.24
2	B	512	VAL	N-CA-C	5.85	117.43	108.71
2	B	316	ILE	CB-CA-C	-5.85	104.39	111.88
2	A	111	ASN	N-CA-C	-5.84	104.11	111.11
2	A	41	ASN	CA-C-N	5.83	127.12	119.84
2	A	41	ASN	C-N-CA	5.83	127.12	119.84
2	B	133	THR	N-CA-C	-5.82	102.04	110.08
2	B	332	VAL	N-CA-C	-5.81	105.18	110.82
2	B	568	VAL	CB-CA-C	-5.81	104.55	110.88
1	C	976	C	C2'-C3'-O3'	5.80	118.20	109.50
2	A	568	VAL	N-CA-C	5.77	119.72	113.43
2	A	503	LEU	CA-C-N	5.75	125.70	119.78
2	A	503	LEU	C-N-CA	5.75	125.70	119.78
2	A	82	ILE	N-CA-CB	5.74	116.35	111.64
1	C	916	U	C4'-C3'-O3'	-5.70	104.44	113.00
2	A	277	PHE	CA-C-N	5.69	126.95	119.84
2	A	277	PHE	C-N-CA	5.69	126.95	119.84
1	C	907	G	C2'-C3'-O3'	5.60	117.91	109.50
2	A	18	ALA	N-CA-C	-5.60	104.26	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	250	SER	N-CA-C	5.59	116.91	108.46
2	A	82	ILE	CB-CA-C	-5.59	106.07	111.05
2	B	195	GLY	N-CA-C	5.59	122.36	112.64
2	B	479	LEU	N-CA-C	-5.57	105.12	111.14
2	B	236	VAL	CB-CA-C	-5.57	102.15	111.29
2	B	15	ARG	N-CA-C	5.56	117.52	109.07
2	A	391	ILE	CB-CA-C	-5.55	104.77	112.04
1	D	961	U	N1-C1'-C2'	5.52	120.28	112.00
1	C	949	C	C4'-C3'-O3'	-5.52	101.13	109.40
2	B	480	ALA	N-CA-C	5.51	115.51	108.24
2	A	15	ARG	N-CA-C	5.49	117.41	109.07
2	A	512	VAL	N-CA-C	5.49	116.89	108.71
2	B	108	GLU	N-CA-C	5.47	117.22	108.41
2	A	470	ARG	N-CA-C	5.46	117.50	108.48
2	B	167	THR	N-CA-C	5.44	116.98	109.15
2	A	415	TYR	N-CA-C	5.41	115.82	109.60
2	B	245	VAL	N-CA-C	-5.39	100.87	109.17
2	B	164	MET	N-CA-C	5.38	118.00	109.50
2	B	154	ARG	N-CA-C	-5.38	104.84	111.40
2	A	224	ARG	CA-C-N	5.34	125.64	119.93
2	A	224	ARG	C-N-CA	5.34	125.64	119.93
2	B	418	ALA	N-CA-C	-5.34	106.61	113.23
2	B	339	HIS	CA-C-N	5.33	126.51	119.84
2	B	339	HIS	C-N-CA	5.33	126.51	119.84
2	A	245	VAL	N-CA-C	-5.32	100.97	109.17
2	B	214	ILE	CB-CA-C	-5.30	105.18	111.81
2	B	94	VAL	N-CA-C	5.25	116.42	108.96
2	A	480	ALA	N-CA-C	5.22	115.03	108.45
2	A	507	ARG	N-CA-C	5.21	118.35	110.64
2	B	256	TYR	N-CA-C	-5.17	105.30	111.03
2	B	171	SER	CB-CA-C	-5.15	109.09	115.89
2	A	360	GLU	CA-C-N	5.15	126.28	119.84
2	A	360	GLU	C-N-CA	5.15	126.28	119.84
2	B	412	SER	N-CA-C	5.13	121.73	110.80
2	B	447	GLN	N-CA-C	5.12	117.99	111.69
2	A	229	PHE	N-CA-C	5.11	121.68	110.80
2	A	311	VAL	N-CA-C	-5.10	105.62	110.42
2	A	251	ALA	N-CA-C	-5.10	107.03	113.20
2	A	395	PHE	N-CA-C	5.09	118.64	112.23
1	C	907	G	O4'-C1'-C2'	5.07	110.87	105.80

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	410	TYR	Sidechain
1	C	911	U	Sidechain
1	C	915	G	Sidechain
1	C	916	U	Sidechain
1	C	923	U	Sidechain
1	C	961	U	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1645	0	835	91	0
1	D	1517	0	772	93	0
2	A	4643	0	4735	554	0
2	B	4643	0	4734	600	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	11	0	0	0	0
5	B	13	0	0	0	0
5	C	9	0	0	1	0
5	D	8	0	0	0	0
All	All	12495	0	11076	1265	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 54.

All (1265) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:525:ASP:HA	2:B:577:VAL:HG23	1.28	1.15
2:A:166:ALA:HB1	2:A:184:LEU:HD12	1.24	1.07
1:D:937:C:H3'	1:D:938:G:H5''	1.06	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:439:TYR:O	2:B:443:ILE:HG12	1.58	1.04
2:A:362:ILE:HD12	2:A:383:ARG:NH2	1.71	1.04
2:A:511:VAL:HG22	2:A:533:PHE:O	1.57	1.04
2:A:40:VAL:HG23	2:A:62:THR:HG22	1.40	1.03
2:A:413:LEU:HD12	2:A:413:LEU:H	1.21	1.02
2:A:82:ILE:HD12	2:A:83:HIS:H	1.22	1.01
2:B:290:GLN:HG3	2:B:291:GLU:H	1.26	1.01
1:C:915:G:H5''	2:B:230:GLY:HA2	1.40	0.99
1:C:953:G:H1	1:C:963:C:H42	0.99	0.98
1:D:937:C:H3'	1:D:938:G:C5'	1.93	0.98
2:A:493:ILE:HG23	2:A:494:GLU:H	1.27	0.97
2:A:477:LYS:HZ2	2:A:478:ARG:H	1.07	0.97
1:C:957:C:H2'	1:C:958:A:H5'	1.46	0.96
2:A:210:VAL:HA	2:A:243:MET:HE1	1.46	0.94
2:B:150:LEU:HD22	2:B:183:ARG:HG2	1.48	0.94
2:B:133:THR:HG22	2:B:145:GLU:OE2	1.67	0.94
2:A:297:LYS:HZ2	2:A:297:LYS:HB3	1.29	0.93
2:A:470:ARG:NH1	2:A:484:ALA:HA	1.82	0.93
2:A:210:VAL:HG22	2:A:243:MET:HE2	1.51	0.92
2:B:547:VAL:CG1	2:B:551:ASP:HA	1.99	0.92
2:A:37:MET:SD	2:A:59:ILE:HD11	2.10	0.92
2:A:198:VAL:HG23	2:A:199:PRO:HD3	1.52	0.92
2:A:321:GLN:HE21	2:B:275:ASP:H	1.06	0.92
1:D:914:A:H8	2:A:232:GLY:H	1.09	0.92
2:B:547:VAL:HG11	2:B:551:ASP:HA	1.52	0.91
2:A:431:PRO:HG3	2:A:469:PRO:HG3	1.52	0.91
2:A:470:ARG:HH12	2:A:484:ALA:HA	1.31	0.91
2:B:290:GLN:HG3	2:B:291:GLU:N	1.83	0.91
2:B:63:ASN:HD22	2:B:66:ILE:H	1.15	0.91
2:A:263:MET:HE2	2:A:308:ASN:HB3	1.50	0.91
2:B:162:ILE:HD12	2:B:163:PRO:HD2	1.53	0.91
2:B:483:ARG:HH22	2:B:558:GLN:HE22	1.12	0.90
2:B:470:ARG:NH1	2:B:484:ALA:HA	1.86	0.90
1:D:914:A:O2'	2:A:250:SER:HB2	1.71	0.90
2:A:200:LEU:HD22	2:A:205:ARG:HD3	1.53	0.90
1:D:968:G:OP1	2:B:478:ARG:HD2	1.71	0.90
2:B:474:VAL:HG13	2:B:479:LEU:HD21	1.52	0.89
2:A:187:MET:HB3	2:A:189:PHE:HE1	1.35	0.89
2:B:286:LYS:HG3	2:B:287:TYR:CD1	2.08	0.89
2:A:321:GLN:NE2	2:B:275:ASP:H	1.69	0.89
2:A:109:VAL:HG21	2:A:114:ILE:HG23	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:406:ARG:H	2:A:406:ARG:HD2	1.39	0.88
2:A:288:THR:OG1	2:A:291:GLU:HG2	1.72	0.87
2:B:355:PHE:HD2	2:B:356:LEU:HD23	1.40	0.87
2:A:433:LYS:HD3	2:A:433:LYS:N	1.88	0.87
2:B:528:ALA:O	2:B:531:VAL:HG23	1.73	0.87
2:B:391:ILE:HG21	2:B:411:LEU:CD2	2.04	0.87
1:C:937:C:H3'	1:C:938:G:H5''	1.55	0.86
2:B:9:LYS:HG3	2:B:571:TYR:CD1	2.10	0.86
2:B:473:LYS:HB3	2:B:478:ARG:HA	1.57	0.86
2:A:110:SER:HB3	2:A:113:GLU:HG3	1.57	0.86
2:A:290:GLN:OE1	2:A:293:ARG:HD2	1.75	0.86
2:B:483:ARG:NH2	2:B:558:GLN:HE22	1.72	0.86
1:D:961:U:H5''	1:D:962:C:H5	1.39	0.86
2:A:215:SER:HA	2:A:218:MET:HE2	1.57	0.86
1:D:937:C:C3'	1:D:938:G:H5''	2.01	0.85
2:A:433:LYS:HD3	2:A:433:LYS:H	1.40	0.85
2:B:370:LYS:HE3	2:B:376:LEU:HD11	1.56	0.85
1:D:915:G:O6	2:A:132:PRO:HB3	1.75	0.85
2:B:538:ILE:HG22	2:B:563:GLY:N	1.92	0.85
2:A:505:TYR:CA	2:A:509:ARG:HH21	1.89	0.85
2:A:548:ASN:HD21	2:A:550:ASN:HB2	1.41	0.84
1:C:953:G:H1	1:C:963:C:N4	1.75	0.84
2:B:45:MET:HE1	2:B:49:PRO:CD	2.07	0.84
2:B:392:ASN:HD21	2:B:407:VAL:HA	1.42	0.83
2:B:525:ASP:HA	2:B:577:VAL:CG2	2.08	0.83
2:A:493:ILE:HG23	2:A:494:GLU:N	1.91	0.83
2:B:517:GLU:HG3	2:B:554:LEU:HD11	1.60	0.83
2:A:187:MET:HB3	2:A:189:PHE:CE1	2.14	0.83
2:B:154:ARG:HG2	2:B:187:MET:HE1	1.57	0.83
2:B:358:GLU:O	2:B:539:ARG:HD3	1.79	0.83
2:A:362:ILE:HA	2:A:383:ARG:NH2	1.94	0.82
2:A:290:GLN:O	2:A:293:ARG:HG2	1.79	0.82
2:A:413:LEU:HD12	2:A:413:LEU:N	1.91	0.82
2:A:117:PHE:CZ	2:A:121:ILE:HD11	2.14	0.82
1:D:913:U:H5''	2:A:256:TYR:OH	1.79	0.81
1:D:968:G:P	2:B:478:ARG:HD2	2.20	0.81
2:B:378:TRP:O	2:B:381:VAL:HG23	1.81	0.81
2:B:534:ALA:N	2:B:567:ILE:HD11	1.96	0.81
2:A:362:ILE:HA	2:A:383:ARG:HH22	1.46	0.81
2:B:45:MET:HE1	2:B:49:PRO:HD3	1.62	0.81
2:B:186:SER:HA	2:B:221:ARG:HH21	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:84:ARG:HA	2:A:84:ARG:CZ	2.11	0.80
2:B:123:VAL:HG22	2:B:124:ASP:H	1.47	0.80
2:A:117:PHE:CE1	2:A:121:ILE:HD11	2.16	0.80
2:A:151:SER:HA	2:A:154:ARG:NH1	1.96	0.80
2:B:223:ASP:HA	2:B:569:PHE:CE2	2.16	0.80
2:B:198:VAL:HA	2:B:201:LEU:HD12	1.62	0.80
2:B:519:PHE:HD1	2:B:519:PHE:H	1.28	0.80
1:D:961:U:H5''	1:D:962:C:C5	2.15	0.80
2:B:286:LYS:HG3	2:B:287:TYR:HD1	1.43	0.80
2:B:561:LEU:HD13	2:B:569:PHE:HD1	1.47	0.80
2:A:336:ALA:HA	2:A:342:LEU:CD2	2.11	0.79
2:B:534:ALA:H	2:B:567:ILE:HD11	1.46	0.79
2:B:265:PRO:HB3	2:B:335:ARG:HE	1.47	0.79
2:A:505:TYR:N	2:A:509:ARG:HH21	1.78	0.79
2:A:439:TYR:O	2:A:443:ILE:HG13	1.82	0.79
2:B:181:ALA:HB1	2:B:220:LEU:HD23	1.64	0.79
2:A:82:ILE:HD12	2:A:83:HIS:N	1.97	0.79
2:A:566:MET:HG2	2:A:574:ALA:HB1	1.64	0.78
2:B:483:ARG:HH22	2:B:558:GLN:NE2	1.81	0.78
2:A:500:HIS:HE1	2:A:551:ASP:OD1	1.66	0.78
2:B:407:VAL:HG21	2:B:417:PHE:CD2	2.17	0.78
1:C:937:C:H3'	1:C:938:G:C5'	2.13	0.78
2:A:181:ALA:HB1	2:A:220:LEU:HD23	1.65	0.78
2:B:166:ALA:HB3	2:B:192:HIS:ND1	1.99	0.78
2:B:250:SER:HB3	2:B:252:SER:OG	1.83	0.78
2:B:392:ASN:HD22	2:B:398:LEU:HD22	1.47	0.77
2:A:563:GLY:HA2	2:A:566:MET:CE	2.14	0.77
2:B:279:CYS:HB3	2:B:284:CYS:SG	2.24	0.77
2:A:477:LYS:NZ	2:A:478:ARG:H	1.82	0.77
2:B:355:PHE:CD2	2:B:356:LEU:HD23	2.17	0.77
2:B:258:LYS:HD2	2:B:301:THR:HG21	1.66	0.77
1:C:915:G:H5''	2:B:230:GLY:CA	2.15	0.77
2:B:146:LEU:HD21	2:B:180:ALA:HB2	1.65	0.77
1:C:937:C:H5'	1:C:938:G:OP2	1.86	0.76
2:A:40:VAL:CG2	2:A:62:THR:HG22	2.15	0.76
1:D:907:G:O2'	1:D:908:U:OP2	2.02	0.76
2:A:155:GLU:O	2:A:159:ILE:HG22	1.84	0.76
2:B:254:ALA:O	2:B:258:LYS:HG2	1.85	0.76
2:A:138:PRO:HD2	2:A:141:GLN:HE21	1.51	0.75
2:B:517:GLU:HG3	2:B:554:LEU:CD1	2.17	0.75
1:C:909:G:N2	2:A:418:ALA:O	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:398:LEU:HD23	2:B:408:SER:CA	2.17	0.75
2:A:74:ARG:O	2:A:78:LEU:HD12	1.86	0.75
2:A:221:ARG:HE	2:A:224:ARG:CD	2.00	0.75
2:A:493:ILE:CG2	2:A:494:GLU:H	1.99	0.75
2:B:227:HIS:HB2	2:B:247:LEU:HB2	1.68	0.75
2:A:232:GLY:HA3	2:A:250:SER:OG	1.86	0.74
1:C:960:G:H2'	1:C:961:U:H5'	1.69	0.74
2:A:286:LYS:HG3	2:A:286:LYS:O	1.86	0.74
2:B:80:LEU:H	2:B:80:LEU:HD23	1.51	0.74
2:A:141:GLN:O	2:A:145:GLU:HB2	1.87	0.74
2:B:57:PHE:HE2	2:B:313:LYS:HG3	1.50	0.74
2:A:504:PRO:C	2:A:509:ARG:HH21	1.96	0.74
2:A:297:LYS:HZ2	2:A:297:LYS:CB	2.00	0.74
1:C:943:G:O2'	1:C:944:G:H5'	1.86	0.74
2:A:101:LEU:HD23	2:A:101:LEU:O	1.87	0.73
2:A:146:LEU:HD21	2:A:180:ALA:HB2	1.69	0.73
2:B:403:ILE:HD12	2:B:403:ILE:N	2.03	0.73
1:C:907:G:H4'	1:C:908:U:C6	2.23	0.73
2:B:561:LEU:HD13	2:B:569:PHE:CD1	2.23	0.73
2:A:500:HIS:ND1	2:A:509:ARG:NH1	2.36	0.73
1:C:907:G:H4'	1:C:908:U:H6	1.54	0.72
2:A:29:LYS:HE2	2:A:83:HIS:HE2	1.53	0.72
2:A:432:THR:HB	2:A:433:LYS:HE2	1.70	0.72
2:B:493:ILE:HG23	2:B:494:GLU:N	2.04	0.72
2:B:559:ALA:O	2:B:560:LEU:HD12	1.89	0.72
2:B:359:PHE:HD2	2:B:359:PHE:N	1.87	0.72
1:C:977:A:N7	2:A:530:PHE:CE1	2.57	0.72
2:B:101:LEU:HD12	2:B:105:GLY:O	1.90	0.72
2:A:138:PRO:HD2	2:A:141:GLN:NE2	2.04	0.72
2:A:386:GLU:HA	2:A:389:LYS:HE3	1.71	0.72
2:B:121:ILE:HD11	2:B:123:VAL:HB	1.71	0.72
1:D:939:A:H2'	1:D:940:G:O4'	1.88	0.72
1:D:957:C:H2'	1:D:958:A:H5'	1.72	0.72
2:A:117:PHE:O	2:A:121:ILE:HG13	1.90	0.72
2:A:579:LYS:HE2	2:A:579:LYS:HA	1.70	0.72
2:B:253:TYR:CD1	2:B:254:ALA:N	2.57	0.72
2:B:539:ARG:O	2:B:542:ASP:HB2	1.90	0.72
2:A:227:HIS:HB2	2:A:247:LEU:HB2	1.71	0.72
1:D:937:C:H5'	1:D:938:G:OP2	1.90	0.72
2:B:36:ILE:HD12	2:B:37:MET:N	2.05	0.72
2:B:206:PHE:CG	2:B:342:LEU:HD12	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:957:C:C2'	1:C:958:A:H5'	2.19	0.71
2:A:560:LEU:HD21	2:A:576:LYS:HD3	1.72	0.71
2:A:513:ASN:OD1	2:A:515:GLU:HB3	1.91	0.71
2:B:8:LEU:C	2:B:8:LEU:HD23	2.15	0.71
2:A:151:SER:HA	2:A:154:ARG:HH12	1.55	0.71
2:A:148:ILE:O	2:A:152:ARG:HG3	1.91	0.71
2:B:45:MET:CE	2:B:49:PRO:HD3	2.21	0.71
2:B:398:LEU:HD23	2:B:408:SER:HA	1.72	0.71
2:A:504:PRO:C	2:A:509:ARG:NH2	2.49	0.70
1:D:911:U:O2'	1:D:912:C:H5'	1.91	0.70
2:A:127:THR:HG23	2:A:165:ASN:HB2	1.72	0.70
2:A:505:TYR:HA	2:A:509:ARG:HH21	1.56	0.70
2:B:111:ASN:C	2:B:111:ASN:HD22	1.99	0.70
2:B:492:GLY:O	2:B:494:GLU:N	2.25	0.70
2:B:141:GLN:O	2:B:145:GLU:HB2	1.92	0.70
2:B:63:ASN:ND2	2:B:66:ILE:HG12	2.07	0.70
2:A:128:PHE:N	2:A:164:MET:HE2	2.07	0.70
1:D:914:A:H8	2:A:232:GLY:N	1.88	0.70
2:A:362:ILE:HG22	2:A:363:THR:HG22	1.72	0.70
2:B:578:ARG:HG3	2:B:578:ARG:HH11	1.56	0.70
2:A:97:GLY:HA2	2:A:100:GLN:OE1	1.91	0.70
2:B:416:PRO:HD2	2:B:417:PHE:CE1	2.26	0.69
1:C:915:G:H2'	1:C:916:U:OP1	1.90	0.69
2:A:483:ARG:HD2	2:A:486:ASP:OD1	1.93	0.69
2:A:111:ASN:O	2:A:115:ILE:HG13	1.92	0.69
1:D:914:A:H1'	2:A:252:SER:HB3	1.73	0.69
2:A:510:VAL:HG23	2:A:546:VAL:HA	1.74	0.69
2:A:548:ASN:ND2	2:A:550:ASN:H	1.91	0.69
2:B:101:LEU:HD21	2:B:131:ILE:HG13	1.75	0.69
2:B:490:THR:HG22	2:B:578:ARG:NH2	2.07	0.69
2:B:358:GLU:HG2	2:B:359:PHE:CD2	2.28	0.69
2:A:68:TYR:HA	2:A:74:ARG:HD3	1.74	0.68
2:A:131:ILE:H	2:A:149:THR:HG23	1.58	0.68
1:C:976:C:OP2	1:C:976:C:H6	1.75	0.68
2:A:274:LEU:HD12	2:A:276:TYR:O	1.93	0.68
2:B:57:PHE:CE2	2:B:313:LYS:HG3	2.27	0.68
2:A:197:VAL:HG21	2:A:228:LEU:HD11	1.74	0.68
2:A:221:ARG:HH21	2:A:224:ARG:HD2	1.58	0.68
2:A:200:LEU:CD2	2:A:205:ARG:HD3	2.23	0.68
2:A:65:TYR:CE1	2:A:107:ILE:HG23	2.29	0.68
2:A:174:THR:HG22	2:A:215:SER:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:168:ILE:HD12	2:A:168:ILE:H	1.58	0.68
2:B:167:THR:OG1	2:B:193:PRO:HG2	1.93	0.68
2:A:82:ILE:HA	2:A:85:MET:HG2	1.76	0.68
2:A:263:MET:HE2	2:A:308:ASN:CB	2.24	0.68
2:A:406:ARG:HD2	2:A:406:ARG:N	2.07	0.68
1:D:976:C:H5''	1:D:977:A:N3	2.09	0.68
2:B:391:ILE:HG21	2:B:411:LEU:HD22	1.76	0.68
2:A:437:ILE:HG23	2:A:438:LYS:N	2.07	0.67
2:B:470:ARG:CZ	2:B:484:ALA:HA	2.23	0.67
2:B:570:GLN:HE21	2:B:570:GLN:HA	1.59	0.67
2:B:103:LYS:HE2	2:B:104:TYR:CE2	2.29	0.67
2:B:181:ALA:HB1	2:B:220:LEU:CD2	2.25	0.67
2:B:392:ASN:HD22	2:B:398:LEU:CD2	2.06	0.67
1:D:977:A:OP2	2:B:530:PHE:HZ	1.77	0.67
2:B:417:PHE:HD1	2:B:417:PHE:H	1.42	0.67
2:B:417:PHE:N	2:B:417:PHE:CD1	2.61	0.67
1:D:967:C:O2'	2:B:478:ARG:NH1	2.26	0.67
2:B:31:ILE:HD11	2:B:59:ILE:HG21	1.76	0.67
2:B:193:PRO:HA	2:B:227:HIS:O	1.94	0.67
2:B:446:TYR:CD1	2:B:446:TYR:C	2.73	0.67
2:B:462:GLU:CD	2:B:471:GLN:HB2	2.19	0.67
2:A:280:SER:O	2:B:281:CYS:HA	1.95	0.67
2:B:31:ILE:CD1	2:B:59:ILE:HG21	2.25	0.67
2:B:70:ASP:HB3	2:B:73:LEU:HD12	1.77	0.67
2:B:330:ARG:HH11	2:B:330:ARG:HB3	1.59	0.67
2:B:370:LYS:HE3	2:B:376:LEU:CD1	2.25	0.67
2:A:510:VAL:CG2	2:A:546:VAL:HA	2.26	0.66
1:C:959:A:H4'	1:C:960:G:OP1	1.95	0.66
2:A:498:ARG:O	2:A:502:VAL:HG23	1.94	0.66
1:D:908:U:OP1	2:B:465:LYS:HG2	1.96	0.66
2:A:140:GLU:HG2	2:A:141:GLN:N	2.09	0.66
2:B:82:ILE:HG23	2:B:83:HIS:N	2.10	0.66
2:B:193:PRO:HB2	2:B:229:PHE:CD2	2.31	0.66
1:C:962:C:H2'	1:C:963:C:C6	2.31	0.66
2:A:99:PHE:HE1	2:A:198:VAL:HG21	1.60	0.66
2:A:239:LEU:HD23	2:A:239:LEU:C	2.20	0.66
2:B:45:MET:HE1	2:B:49:PRO:HD2	1.75	0.66
2:B:186:SER:CA	2:B:221:ARG:HH21	2.09	0.66
1:D:913:U:O3'	2:A:256:TYR:HE2	1.79	0.66
2:B:185:SER:OG	2:B:221:ARG:HD3	1.96	0.66
2:B:253:TYR:CE1	2:B:254:ALA:HB2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:PRO:C	2:B:403:ILE:HD12	2.21	0.65
2:A:8:LEU:HD12	2:A:190:GLU:HB2	1.77	0.65
2:B:287:TYR:HE2	2:B:295:MET:HE1	1.59	0.65
1:C:961:U:O2'	1:C:962:C:OP1	2.09	0.65
2:A:131:ILE:O	2:A:169:GLN:HG2	1.96	0.65
2:A:328:LEU:O	2:A:332:VAL:HG23	1.97	0.65
2:A:362:ILE:HD12	2:A:383:ARG:CZ	2.26	0.65
2:B:123:VAL:HG22	2:B:124:ASP:N	2.10	0.65
2:B:359:PHE:N	2:B:359:PHE:CD2	2.58	0.65
2:B:111:ASN:OD1	2:B:152:ARG:HB3	1.96	0.65
2:A:36:ILE:HG13	2:A:248:PHE:HB2	1.77	0.65
2:B:358:GLU:OE2	2:B:359:PHE:HE2	1.79	0.65
1:D:916:U:C5	2:A:41:ASN:HB2	2.32	0.65
1:C:968:G:O5'	2:A:478:ARG:HD3	1.96	0.65
2:B:53:GLU:HB2	2:B:88:TYR:HE1	1.62	0.65
2:A:492:GLY:O	2:A:494:GLU:N	2.30	0.64
2:B:493:ILE:CG2	2:B:494:GLU:N	2.60	0.64
2:B:165:ASN:OD1	2:B:191:ILE:CG2	2.46	0.64
1:C:977:A:N7	2:A:530:PHE:HE1	1.96	0.64
2:B:53:GLU:HB2	2:B:88:TYR:CE1	2.32	0.64
2:A:233:HIS:ND1	2:A:234:PRO:HD2	2.13	0.64
2:B:414:THR:HG23	2:B:487:GLY:O	1.97	0.64
2:B:497:LYS:HD3	2:B:553:LEU:HD23	1.78	0.64
1:D:909:G:OP1	2:B:466:THR:HG21	1.97	0.64
2:B:446:TYR:C	2:B:446:TYR:HD1	2.06	0.64
2:A:210:VAL:HG22	2:A:243:MET:CE	2.26	0.64
2:B:306:LEU:HA	2:B:309:LEU:HD12	1.80	0.64
2:A:500:HIS:CE1	2:A:551:ASP:OD1	2.50	0.64
1:C:908:U:OP1	2:A:465:LYS:HE3	1.97	0.63
2:B:63:ASN:HD22	2:B:66:ILE:N	1.92	0.63
2:B:418:ALA:HB3	2:B:419:GLN:OE1	1.99	0.63
2:B:553:LEU:C	2:B:554:LEU:HD23	2.22	0.63
2:A:281:CYS:HA	2:B:280:SER:O	1.98	0.63
2:B:290:GLN:HG3	2:B:291:GLU:HG3	1.79	0.63
2:B:358:GLU:HA	2:B:539:ARG:NE	2.13	0.63
2:B:460:LYS:HZ3	2:B:475:ASN:H	1.47	0.63
2:A:391:ILE:HD12	2:A:391:ILE:H	1.64	0.63
1:C:929:C:O2'	1:C:930:G:H5'	1.99	0.63
2:A:10:PHE:CD2	2:A:225:PRO:HG3	2.34	0.63
2:A:483:ARG:NH1	2:A:486:ASP:OD1	2.31	0.63
2:A:159:ILE:HG13	2:A:159:ILE:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:537:GLY:HA2	2:A:539:ARG:NH1	2.14	0.62
2:B:131:ILE:CG2	2:B:145:GLU:HG2	2.29	0.62
1:D:962:C:H2'	1:D:963:C:C6	2.34	0.62
2:A:187:MET:CB	2:A:189:PHE:HE1	2.11	0.62
2:A:513:ASN:HA	2:A:532:ILE:HD11	1.81	0.62
2:A:168:ILE:HD12	2:A:168:ILE:N	2.14	0.62
2:B:553:LEU:O	2:B:581:VAL:HG11	1.99	0.62
1:D:916:U:OP1	2:A:99:PHE:HB3	1.98	0.62
2:A:207:ARG:HD2	2:A:348:ARG:NH1	2.13	0.62
2:B:115:ILE:HD13	2:B:115:ILE:O	2.00	0.62
2:B:165:ASN:OD1	2:B:191:ILE:HG22	2.00	0.62
2:B:80:LEU:HD23	2:B:80:LEU:N	2.14	0.62
2:B:98:SER:O	2:B:101:LEU:HB3	1.99	0.62
2:B:381:VAL:HG12	2:B:404:PHE:CE2	2.35	0.62
2:A:581:VAL:HG13	2:A:582:GLU:HG3	1.82	0.62
2:B:281:CYS:O	2:B:285:SER:HB2	1.99	0.62
2:A:242:ALA:HB2	2:A:328:LEU:HD21	1.82	0.61
2:A:114:ILE:HD11	2:A:129:LEU:HB2	1.82	0.61
2:B:12:ILE:HG22	2:B:12:ILE:O	2.00	0.61
2:B:10:PHE:CG	2:B:225:PRO:HG3	2.36	0.61
2:B:449:GLY:HA3	2:B:507:ARG:HH12	1.65	0.61
2:A:82:ILE:HG23	2:A:121:ILE:HG22	1.81	0.61
2:A:365:LYS:N	2:A:365:LYS:HD3	2.14	0.61
2:B:468:MET:HE3	2:B:470:ARG:NH2	2.16	0.61
2:B:473:LYS:HB3	2:B:478:ARG:CA	2.28	0.61
1:C:950:C:O5'	1:C:950:C:H6	1.83	0.61
2:A:578:ARG:O	2:A:579:LYS:HE2	2.01	0.61
2:B:150:LEU:O	2:B:154:ARG:HG3	2.00	0.61
2:B:287:TYR:HE2	2:B:295:MET:CE	2.14	0.61
2:B:547:VAL:HG22	2:B:553:LEU:HA	1.83	0.61
2:A:197:VAL:O	2:A:200:LEU:HB2	2.01	0.61
2:B:197:VAL:CG1	2:B:209:VAL:HG22	2.31	0.61
2:B:473:LYS:CB	2:B:478:ARG:HA	2.31	0.61
2:A:287:TYR:HA	2:A:291:GLU:OE1	2.00	0.60
2:B:36:ILE:HG22	2:B:316:ILE:CD1	2.31	0.60
2:B:411:LEU:HD11	2:B:446:TYR:CD2	2.36	0.60
2:A:290:GLN:O	2:A:293:ARG:CG	2.49	0.60
2:B:459:ALA:HA	2:B:474:VAL:HG12	1.83	0.60
2:B:563:GLY:O	2:B:565:GLU:N	2.34	0.60
2:A:370:LYS:HE3	2:A:423:GLU:OE1	2.00	0.60
2:B:130:ASP:OD2	2:B:167:THR:HB	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:135:PRO:HG2	2:B:200:LEU:HD13	1.83	0.60
2:B:286:LYS:HG3	2:B:287:TYR:CE1	2.36	0.60
2:B:562:SER:O	2:B:565:GLU:HB2	2.02	0.60
2:A:82:ILE:HG23	2:A:121:ILE:CG2	2.31	0.60
2:B:507:ARG:C	2:B:508:MET:HG2	2.27	0.60
2:B:570:GLN:HA	2:B:570:GLN:NE2	2.16	0.60
2:B:162:ILE:CD1	2:B:163:PRO:HD2	2.28	0.60
2:A:529:LYS:HG2	2:A:570:GLN:HG3	1.83	0.60
2:B:168:ILE:HD11	2:B:220:LEU:HD11	1.84	0.60
2:A:307:HIS:CD2	2:A:308:ASN:ND2	2.70	0.59
2:B:21:ILE:HA	2:B:33:THR:O	2.02	0.59
2:B:290:GLN:O	2:B:294:GLU:HG2	2.02	0.59
2:B:462:GLU:HG2	2:B:471:GLN:O	2.02	0.59
2:A:68:TYR:HA	2:A:74:ARG:CD	2.32	0.59
2:A:168:ILE:HD11	2:A:192:HIS:HB3	1.83	0.59
2:A:271:LEU:HD21	2:A:292:LEU:HD23	1.84	0.59
2:A:477:LYS:HA	2:A:477:LYS:HZ3	1.66	0.59
2:B:450:GLU:O	2:B:507:ARG:NH2	2.34	0.59
2:B:63:ASN:ND2	2:B:66:ILE:H	1.92	0.59
2:B:422:ALA:O	2:B:423:GLU:C	2.44	0.59
2:B:191:ILE:HG12	2:B:225:PRO:HB2	1.83	0.59
2:B:316:ILE:HG22	2:B:320:LYS:HE3	1.84	0.59
2:B:511:VAL:CG1	2:B:532:ILE:HG22	2.32	0.59
1:D:909:G:C5	2:B:428:ILE:HD11	2.38	0.59
2:A:118:GLN:O	2:A:123:VAL:HG22	2.02	0.59
2:A:217:LYS:HE3	2:A:244:GLY:HA3	1.84	0.59
2:B:480:ALA:HB2	2:B:491:LEU:HD23	1.83	0.59
2:B:63:ASN:HB3	2:B:66:ILE:HG13	1.83	0.59
2:B:156:ALA:HA	2:B:159:ILE:HG22	1.85	0.59
2:B:315:GLU:O	2:B:319:VAL:HG23	2.02	0.59
2:A:110:SER:O	2:A:114:ILE:HG12	2.02	0.59
2:A:193:PRO:HA	2:A:227:HIS:O	2.02	0.59
2:A:206:PHE:HE1	2:A:236:VAL:HG13	1.67	0.59
2:A:169:GLN:HE22	2:A:195:GLY:C	2.10	0.59
2:B:410:TYR:H	2:B:410:TYR:HD1	1.49	0.59
2:B:460:LYS:NZ	2:B:475:ASN:H	2.00	0.59
2:B:490:THR:HG22	2:B:578:ARG:HH21	1.67	0.59
2:A:127:THR:C	2:A:164:MET:HE2	2.27	0.59
2:B:159:ILE:HG12	2:B:159:ILE:O	2.03	0.59
2:B:166:ALA:HB3	2:B:192:HIS:CE1	2.38	0.59
2:B:175:ASP:OD2	2:B:176:LEU:HD23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:MET:HE2	2:B:349:LEU:HD13	1.83	0.58
2:B:259:ASP:OD2	2:B:261:ARG:NH1	2.36	0.58
2:B:548:ASN:OD1	2:B:552:GLU:N	2.33	0.58
1:C:915:G:H1'	2:B:229:PHE:CD1	2.38	0.58
2:A:215:SER:HA	2:A:218:MET:CE	2.31	0.58
2:A:240:ALA:O	2:A:243:MET:HB2	2.02	0.58
2:B:403:ILE:HD11	2:B:422:ALA:HB2	1.84	0.58
2:B:432:THR:O	2:B:434:GLU:N	2.36	0.58
2:A:546:VAL:HG12	2:A:554:LEU:HB2	1.85	0.58
2:B:113:GLU:O	2:B:116:GLU:HG2	2.04	0.58
2:B:168:ILE:HD11	2:B:220:LEU:HD21	1.84	0.58
1:C:931:C:H1'	5:C:28:HOH:O	2.02	0.58
2:A:295:MET:SD	2:A:296:PRO:CD	2.91	0.58
1:C:918:G:H4'	2:B:41:ASN:HD21	1.67	0.58
2:A:97:GLY:O	2:A:100:GLN:HB2	2.03	0.58
2:B:24:LEU:HB3	2:B:31:ILE:HG23	1.86	0.58
2:B:431:PRO:HG3	2:B:469:PRO:HG3	1.86	0.58
1:D:914:A:C8	2:A:232:GLY:N	2.67	0.58
2:A:433:LYS:N	2:A:433:LYS:CD	2.61	0.58
2:A:539:ARG:O	2:A:542:ASP:HB2	2.04	0.58
2:A:279:CYS:SG	2:A:280:SER:N	2.76	0.58
2:A:432:THR:O	2:A:434:GLU:N	2.36	0.58
2:A:391:ILE:HD12	2:A:391:ILE:N	2.19	0.58
2:B:45:MET:HE3	2:B:48:GLU:HA	1.86	0.58
2:B:163:PRO:HA	2:B:190:GLU:CD	2.29	0.58
2:B:268:THR:O	2:B:269:LYS:HD3	2.04	0.58
2:A:468:MET:HE3	2:A:470:ARG:NH2	2.19	0.57
2:B:31:ILE:HG12	2:B:32:GLU:N	2.19	0.57
2:B:435:ASP:O	2:B:437:ILE:N	2.37	0.57
2:B:460:LYS:O	2:B:472:VAL:HA	2.03	0.57
2:A:137:ALA:HB1	2:A:141:GLN:NE2	2.19	0.57
2:A:270:ARG:O	2:A:271:LEU:C	2.47	0.57
2:A:516:ALA:C	2:A:518:PRO:HD2	2.29	0.57
1:D:959:A:H2'	1:D:961:U:OP2	2.04	0.57
2:A:321:GLN:O	2:A:325:GLU:HG3	2.04	0.57
1:D:946:G:O2'	1:D:947:G:C8	2.58	0.57
2:A:21:ILE:HA	2:A:33:THR:O	2.04	0.57
2:A:260:ASP:OD1	2:A:300:ARG:HD2	2.05	0.57
2:A:431:PRO:HB3	2:A:439:TYR:CE1	2.40	0.57
2:B:204:TYR:CD1	2:B:206:PHE:HE1	2.22	0.57
2:A:166:ALA:HB1	2:A:184:LEU:CD1	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:319:VAL:O	2:B:322:ALA:HB3	2.04	0.57
2:A:237:PHE:N	2:A:237:PHE:CD2	2.70	0.57
2:A:221:ARG:HE	2:A:224:ARG:HD2	1.69	0.57
2:B:496:ALA:HB2	2:B:556:THR:OG1	2.04	0.57
2:A:61:ILE:HA	2:A:93:GLU:O	2.05	0.57
2:A:307:HIS:CD2	2:A:308:ASN:HD22	2.23	0.57
2:A:348:ARG:HH11	2:A:348:ARG:HB2	1.68	0.57
2:B:227:HIS:HB2	2:B:247:LEU:CB	2.33	0.57
2:B:232:GLY:HA3	2:B:250:SER:HB2	1.86	0.57
1:D:967:C:H6	1:D:967:C:O5'	1.88	0.57
2:B:135:PRO:HG2	2:B:200:LEU:CD1	2.35	0.57
1:C:926:C:H2'	1:C:927:G:C8	2.40	0.56
2:A:560:LEU:C	2:A:561:LEU:HD12	2.30	0.56
2:B:112:ARG:O	2:B:115:ILE:HG22	2.04	0.56
2:B:410:TYR:CD1	2:B:410:TYR:N	2.73	0.56
1:C:960:G:N3	1:C:960:G:H5'	2.20	0.56
2:A:65:TYR:HB2	2:A:96:SER:O	2.05	0.56
2:A:74:ARG:O	2:A:77:ALA:HB3	2.06	0.56
2:A:140:GLU:HA	2:A:143:VAL:HG23	1.87	0.56
2:B:512:VAL:HG22	2:B:547:VAL:O	2.05	0.56
1:C:965:C:O2'	1:C:966:G:H5'	2.06	0.56
2:A:231:ALA:O	2:A:248:PHE:HB3	2.05	0.56
2:A:474:VAL:HG11	2:A:498:ARG:HH12	1.70	0.56
2:B:217:LYS:HD2	2:B:244:GLY:HA3	1.87	0.56
1:C:915:G:C2'	1:C:916:U:OP1	2.54	0.56
2:A:37:MET:CG	2:A:59:ILE:HD11	2.35	0.56
2:A:567:ILE:HG22	2:A:568:VAL:CG1	2.36	0.56
2:B:511:VAL:HG12	2:B:532:ILE:HG22	1.87	0.56
2:A:297:LYS:NZ	2:A:301:THR:HG23	2.21	0.56
2:A:315:GLU:O	2:A:318:ARG:HB3	2.04	0.56
2:B:414:THR:OG1	2:B:443:ILE:HD12	2.06	0.56
2:A:477:LYS:NZ	2:A:477:LYS:HA	2.20	0.56
2:A:511:VAL:HG12	2:A:547:VAL:CG2	2.35	0.56
2:B:36:ILE:HG22	2:B:316:ILE:HD11	1.87	0.56
2:B:61:ILE:HA	2:B:93:GLU:O	2.06	0.56
1:C:914:A:H8	2:B:232:GLY:H	1.51	0.56
2:A:82:ILE:CD1	2:A:83:HIS:ND1	2.69	0.56
2:B:246:ASP:O	2:B:247:LEU:HD12	2.05	0.56
2:B:124:ASP:C	2:B:162:ILE:HD11	2.30	0.56
2:B:191:ILE:CG1	2:B:225:PRO:HB2	2.36	0.56
2:B:497:LYS:NZ	2:B:553:LEU:H	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:946:G:O2'	1:C:947:G:C8	2.57	0.56
1:D:952:G:N2	1:D:965:C:C2	2.74	0.56
2:B:186:SER:HA	2:B:221:ARG:NH2	2.20	0.56
2:B:231:ALA:O	2:B:248:PHE:HB3	2.06	0.56
2:B:290:GLN:HA	2:B:293:ARG:HH12	1.70	0.56
2:B:175:ASP:CG	2:B:176:LEU:HD23	2.31	0.55
2:A:8:LEU:HD12	2:A:190:GLU:CB	2.36	0.55
1:C:937:C:C5	1:C:938:G:C8	2.94	0.55
2:A:262:TYR:CZ	2:A:307:HIS:CE1	2.95	0.55
2:B:8:LEU:HG	2:B:26:VAL:HG22	1.86	0.55
2:B:396:GLY:O	2:B:408:SER:HB2	2.06	0.55
2:B:493:ILE:CG2	2:B:494:GLU:H	2.19	0.55
1:D:952:G:N2	1:D:965:C:O2	2.39	0.55
2:A:422:ALA:O	2:A:423:GLU:C	2.49	0.55
2:A:519:PHE:O	2:A:520:ALA:C	2.48	0.55
1:D:976:C:O2'	1:D:977:A:OP2	2.17	0.55
2:A:297:LYS:CB	2:A:297:LYS:NZ	2.70	0.55
2:A:563:GLY:HA2	2:A:566:MET:HE3	1.89	0.55
2:B:392:ASN:ND2	2:B:407:VAL:HA	2.18	0.55
1:C:936:A:N1	1:C:937:C:C5	2.75	0.55
2:A:535:ASP:HB3	2:A:538:ILE:HG13	1.88	0.55
2:B:53:GLU:OE2	2:B:89:ASN:OD1	2.25	0.55
2:B:414:THR:HG22	2:B:488:LEU:HD13	1.87	0.55
2:B:31:ILE:HG12	2:B:32:GLU:H	1.72	0.55
2:B:329:TRP:HA	2:B:332:VAL:HG23	1.88	0.55
2:A:63:ASN:OD1	2:A:66:ILE:HG13	2.07	0.55
2:B:286:LYS:O	2:B:287:TYR:CD1	2.60	0.55
2:B:476:GLY:O	2:B:478:ARG:NH2	2.40	0.55
1:C:951:G:H2'	1:C:952:G:H8	1.72	0.55
1:D:946:G:O2'	1:D:947:G:H8	1.90	0.55
2:B:131:ILE:HG21	2:B:145:GLU:HG2	1.89	0.55
2:B:454:ARG:HA	2:B:457:ASP:CG	2.32	0.55
2:B:519:PHE:CD1	2:B:519:PHE:N	2.68	0.55
2:B:146:LEU:CD2	2:B:180:ALA:HB2	2.37	0.54
2:B:367:ALA:HB1	2:B:419:GLN:O	2.07	0.54
2:A:325:GLU:O	2:A:365:LYS:HG2	2.07	0.54
2:B:33:THR:HA	2:B:34:PRO:C	2.32	0.54
2:B:571:TYR:N	2:B:571:TYR:CD2	2.73	0.54
1:C:938:G:N2	2:B:207:ARG:HH12	2.05	0.54
2:A:210:VAL:HG13	2:A:243:MET:SD	2.48	0.54
2:B:412:SER:O	2:B:428:ILE:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:ARG:NH2	2:B:175:ASP:OD1	2.41	0.54
2:B:223:ASP:HA	2:B:569:PHE:HE2	1.71	0.54
2:B:470:ARG:HH12	2:B:484:ALA:HA	1.70	0.54
2:B:388:ALA:O	2:B:392:ASN:OD1	2.26	0.54
2:B:403:ILE:N	2:B:403:ILE:CD1	2.70	0.54
2:A:435:ASP:O	2:A:437:ILE:N	2.41	0.54
2:B:112:ARG:HA	2:B:115:ILE:HG22	1.89	0.54
2:B:198:VAL:CA	2:B:201:LEU:HD12	2.35	0.54
2:B:360:GLU:HB3	2:B:383:ARG:HH22	1.72	0.54
2:B:403:ILE:HD11	2:B:422:ALA:CB	2.38	0.54
2:B:335:ARG:HH11	2:B:335:ARG:HG2	1.73	0.54
2:B:337:ARG:HH22	2:B:372:SER:HB2	1.72	0.54
1:D:917:U:O2'	2:A:43:LYS:NZ	2.40	0.54
2:A:295:MET:SD	2:A:296:PRO:HD2	2.48	0.54
2:A:407:VAL:HG21	2:A:417:PHE:CD2	2.43	0.54
2:A:407:VAL:HG21	2:A:417:PHE:CE2	2.43	0.54
2:A:529:LYS:CG	2:A:570:GLN:HG3	2.37	0.54
2:A:559:ALA:O	2:A:560:LEU:HD23	2.08	0.54
2:B:29:LYS:NZ	2:B:83:HIS:CD2	2.76	0.54
2:B:270:ARG:O	2:B:273:GLU:HB3	2.08	0.54
2:A:403:ILE:CD1	2:A:420:SER:HB2	2.38	0.54
2:B:98:SER:HB2	2:B:132:PRO:HD3	1.90	0.54
2:B:270:ARG:O	2:B:271:LEU:C	2.50	0.54
2:B:507:ARG:O	2:B:508:MET:HG2	2.07	0.54
1:C:903:G:C2	1:C:972:C:O2	2.60	0.53
1:D:953:G:N2	1:D:964:C:C2	2.76	0.53
2:A:37:MET:HG2	2:A:59:ILE:HD11	1.89	0.53
1:D:953:G:H2'	1:D:954:G:O4'	2.08	0.53
2:A:563:GLY:O	2:A:565:GLU:N	2.41	0.53
2:B:13:LYS:CG	2:B:23:LYS:HG3	2.39	0.53
2:B:455:ALA:HB2	2:B:502:VAL:HG11	1.90	0.53
2:A:295:MET:SD	2:A:296:PRO:HD3	2.48	0.53
2:B:178:ARG:NH1	2:B:178:ARG:HB2	2.24	0.53
2:B:330:ARG:NH1	2:B:331:LEU:N	2.57	0.53
2:B:358:GLU:HA	2:B:539:ARG:CZ	2.39	0.53
2:B:437:ILE:HG23	2:B:438:LYS:N	2.23	0.53
2:B:554:LEU:C	2:B:581:VAL:HG13	2.34	0.53
1:C:917:U:C6	2:B:104:TYR:CE1	2.96	0.53
2:B:131:ILE:CG2	2:B:131:ILE:O	2.56	0.53
2:B:167:THR:OG1	2:B:193:PRO:CG	2.56	0.53
2:B:270:ARG:HH12	2:B:272:ASP:CG	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:912:C:H4'	2:B:204:TYR:CE2	2.44	0.53
1:D:915:G:H5''	2:A:230:GLY:CA	2.38	0.53
2:B:74:ARG:O	2:B:77:ALA:HB3	2.08	0.53
2:A:185:SER:O	2:A:224:ARG:NH2	2.42	0.53
2:B:20:ARG:N	2:B:20:ARG:CD	2.72	0.53
2:B:162:ILE:HG13	2:B:163:PRO:N	2.24	0.53
2:B:478:ARG:H	2:B:478:ARG:HE	1.54	0.53
1:C:938:G:H21	2:B:207:ARG:HH22	1.56	0.53
2:A:37:MET:HG2	2:A:59:ILE:CD1	2.39	0.53
2:A:154:ARG:O	2:A:157:GLU:HB3	2.09	0.53
2:A:339:HIS:HD2	2:A:341:LYS:H	1.56	0.53
2:A:566:MET:HG2	2:A:574:ALA:CB	2.36	0.53
2:B:454:ARG:HA	2:B:457:ASP:OD1	2.09	0.53
2:A:339:HIS:CD2	2:A:341:LYS:H	2.27	0.53
2:B:24:LEU:O	2:B:31:ILE:HG22	2.09	0.53
2:B:297:LYS:O	2:B:298:GLU:C	2.50	0.53
2:B:82:ILE:HG23	2:B:83:HIS:H	1.74	0.53
2:B:101:LEU:O	2:B:105:GLY:HA2	2.09	0.53
2:B:127:THR:OG1	2:B:165:ASN:HB2	2.09	0.53
2:B:398:LEU:HA	2:B:408:SER:HA	1.91	0.53
2:B:471:GLN:HG3	2:B:481:THR:HG23	1.90	0.53
1:C:970:G:H2'	1:C:971:C:C6	2.45	0.52
2:A:67:ILE:HG23	2:A:73:LEU:HB3	1.90	0.52
1:D:957:C:C2'	1:D:958:A:H5'	2.38	0.52
2:A:242:ALA:HB2	2:A:328:LEU:CD2	2.40	0.52
2:B:246:ASP:C	2:B:247:LEU:HD12	2.34	0.52
2:B:519:PHE:O	2:B:520:ALA:C	2.51	0.52
1:C:934:U:H2'	1:C:936:A:H2	1.74	0.52
1:C:967:C:O5'	1:C:967:C:H6	1.92	0.52
2:A:156:ALA:HA	2:A:159:ILE:CG2	2.38	0.52
2:A:258:LYS:HA	2:A:301:THR:HG21	1.91	0.52
2:B:121:ILE:CD1	2:B:123:VAL:HB	2.38	0.52
2:B:455:ALA:CB	2:B:499:LEU:HD12	2.40	0.52
1:C:976:C:H4'	1:C:977:A:OP2	2.08	0.52
2:A:16:ASP:OD2	2:A:17:GLY:N	2.36	0.52
2:A:112:ARG:HG2	2:A:116:GLU:OE1	2.09	0.52
2:A:346:TYR:CZ	2:A:350:LEU:HD11	2.45	0.52
2:A:423:GLU:OE2	2:A:423:GLU:N	2.42	0.52
2:B:111:ASN:C	2:B:111:ASN:ND2	2.66	0.52
2:B:448:PHE:HA	2:B:508:MET:HE1	1.90	0.52
2:A:392:ASN:OD1	2:A:408:SER:N	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:403:ILE:HD12	2:A:420:SER:HB2	1.92	0.52
2:A:365:LYS:HD3	2:A:365:LYS:H	1.73	0.52
2:A:548:ASN:OD1	2:A:552:GLU:HB2	2.10	0.52
2:A:567:ILE:HG22	2:A:568:VAL:HG13	1.92	0.52
2:A:130:ASP:C	2:A:131:ILE:HD13	2.35	0.52
2:A:131:ILE:HG21	2:A:145:GLU:HG2	1.90	0.52
2:A:272:ASP:HA	2:A:293:ARG:HH12	1.75	0.52
2:B:223:ASP:CA	2:B:569:PHE:CE2	2.91	0.52
2:B:554:LEU:HD23	2:B:554:LEU:N	2.25	0.52
2:A:182:ARG:HA	2:A:185:SER:OG	2.10	0.52
2:A:469:PRO:O	2:A:482:VAL:HB	2.10	0.52
2:B:548:ASN:HB3	2:B:554:LEU:HD11	1.92	0.52
1:D:962:C:N3	1:D:963:C:N4	2.58	0.51
2:A:19:GLY:HA2	2:A:244:GLY:HA2	1.92	0.51
2:A:516:ALA:C	2:A:518:PRO:CD	2.83	0.51
2:B:29:LYS:NZ	2:B:83:HIS:NE2	2.57	0.51
2:B:287:TYR:CE2	2:B:295:MET:HE1	2.43	0.51
2:B:355:PHE:HD2	2:B:356:LEU:CD2	2.18	0.51
2:A:108:GLU:O	2:A:109:VAL:HB	2.10	0.51
2:A:299:GLU:HA	2:A:299:GLU:OE2	2.11	0.51
2:B:110:SER:OG	2:B:113:GLU:HG3	2.10	0.51
2:B:410:TYR:HE2	2:B:438:LYS:HD3	1.74	0.51
2:A:268:THR:O	2:A:269:LYS:HD3	2.10	0.51
2:B:290:GLN:CG	2:B:291:GLU:H	2.09	0.51
2:B:407:VAL:HG21	2:B:417:PHE:CE2	2.45	0.51
2:B:315:GLU:O	2:B:318:ARG:HB2	2.10	0.51
2:A:9:LYS:HG3	2:A:571:TYR:CD2	2.45	0.51
2:A:365:LYS:H	2:A:365:LYS:CD	2.24	0.51
2:A:84:ARG:NH2	2:A:87:ASP:HA	2.26	0.51
2:A:519:PHE:O	2:A:522:LYS:N	2.43	0.51
2:A:9:LYS:O	2:A:24:LEU:HD12	2.11	0.51
2:A:269:LYS:HB3	2:A:274:LEU:HD21	1.93	0.51
2:A:505:TYR:N	2:A:509:ARG:NH2	2.52	0.51
2:B:64:SER:HB3	2:B:94:VAL:HG11	1.92	0.51
2:B:168:ILE:CD1	2:B:220:LEU:HD11	2.41	0.51
2:B:176:LEU:HD23	2:B:176:LEU:N	2.25	0.51
2:B:197:VAL:O	2:B:200:LEU:HB2	2.11	0.51
2:B:217:LYS:HD2	2:B:244:GLY:O	2.11	0.51
2:B:506:PRO:O	2:B:535:ASP:HB2	2.11	0.51
1:D:953:G:C2	1:D:964:C:C2	2.99	0.51
2:A:45:MET:HE3	2:A:48:GLU:OE1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:80:LEU:O	2:A:84:ARG:HB2	2.11	0.51
2:A:258:LYS:HA	2:A:301:THR:CG2	2.41	0.51
2:A:287:TYR:CD2	2:A:292:LEU:HD12	2.46	0.51
2:B:148:ILE:O	2:B:152:ARG:HG3	2.10	0.51
2:B:441:MET:O	2:B:444:ALA:HB3	2.11	0.51
1:D:936:A:H3'	1:D:936:A:N3	2.26	0.51
1:D:976:C:C2	2:B:527:PHE:HD2	2.29	0.51
2:A:454:ARG:C	2:A:456:PHE:H	2.18	0.51
2:B:12:ILE:HG13	2:B:20:ARG:CG	2.41	0.51
2:B:131:ILE:HG23	2:B:145:GLU:HG2	1.93	0.51
2:A:47:VAL:HB	2:A:51:GLU:OE1	2.11	0.51
2:B:311:VAL:O	2:B:312:ILE:C	2.54	0.51
2:A:31:ILE:HG21	2:A:59:ILE:HG22	1.93	0.50
2:A:286:LYS:O	2:A:286:LYS:CG	2.59	0.50
1:D:932:C:C2	1:D:941:G:N2	2.79	0.50
1:D:962:C:H2'	1:D:963:C:C5	2.46	0.50
2:A:357:GLU:CD	2:A:357:GLU:C	2.79	0.50
2:A:525:ASP:HA	2:A:577:VAL:HG23	1.93	0.50
2:A:562:SER:O	2:A:565:GLU:HB2	2.11	0.50
2:B:79:GLU:HB3	2:B:80:LEU:HD23	1.92	0.50
2:B:404:PHE:N	2:B:404:PHE:CD1	2.78	0.50
1:D:914:A:H2	2:A:202:GLU:HA	1.76	0.50
2:A:144:LYS:O	2:A:148:ILE:HG13	2.12	0.50
2:A:287:TYR:HD2	2:A:292:LEU:HB2	1.75	0.50
2:B:82:ILE:CG2	2:B:83:HIS:N	2.74	0.50
2:B:253:TYR:CD1	2:B:253:TYR:C	2.88	0.50
2:B:538:ILE:HG22	2:B:563:GLY:H	1.74	0.50
2:A:168:ILE:H	2:A:168:ILE:CD1	2.24	0.50
2:A:401:HIS:N	2:A:405:GLY:O	2.36	0.50
2:A:517:GLU:N	2:A:518:PRO:CD	2.75	0.50
2:B:252:SER:HB2	2:B:263:MET:HE1	1.93	0.50
2:B:337:ARG:NH1	2:B:343:TYR:CE1	2.79	0.50
2:B:358:GLU:HG2	2:B:359:PHE:HD2	1.75	0.50
2:A:297:LYS:O	2:A:298:GLU:C	2.53	0.50
2:A:382:ARG:NH1	2:A:382:ARG:HG3	2.25	0.50
2:B:454:ARG:C	2:B:456:PHE:H	2.19	0.50
1:C:907:G:O2'	1:C:908:U:OP2	2.21	0.50
2:B:330:ARG:HH12	2:B:331:LEU:CA	2.24	0.50
2:B:434:GLU:CD	2:B:434:GLU:H	2.18	0.50
1:C:922:A:H2'	1:C:923:U:O4'	2.11	0.50
1:C:959:A:C2	1:C:962:C:C5	3.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:916:U:OP1	2:A:99:PHE:CD2	2.64	0.50
2:A:279:CYS:SG	2:A:281:CYS:SG	3.10	0.50
2:A:174:THR:HG22	2:A:215:SER:CB	2.41	0.50
2:A:101:LEU:O	2:A:105:GLY:HA2	2.12	0.50
2:A:359:PHE:N	2:A:359:PHE:CD1	2.79	0.50
2:A:431:PRO:HB3	2:A:439:TYR:CD1	2.46	0.50
2:A:437:ILE:CG2	2:A:438:LYS:N	2.73	0.50
2:B:76:LYS:HE2	2:B:85:MET:HG3	1.94	0.50
2:B:214:ILE:O	2:B:215:SER:C	2.55	0.50
2:B:414:THR:CG2	2:B:488:LEU:HD13	2.42	0.50
2:B:431:PRO:CG	2:B:469:PRO:HD3	2.42	0.50
2:A:38:PRO:HD2	2:A:60:ILE:HG22	1.94	0.49
2:A:381:VAL:HG13	2:A:404:PHE:CE2	2.47	0.49
2:B:516:ALA:C	2:B:518:PRO:HD2	2.36	0.49
2:A:339:HIS:CD2	2:A:339:HIS:C	2.90	0.49
2:A:401:HIS:CD2	2:A:426:PHE:CD1	3.00	0.49
2:B:10:PHE:CD1	2:B:24:LEU:HD12	2.47	0.49
2:B:400:GLU:HA	2:B:405:GLY:O	2.12	0.49
1:D:959:A:H1'	1:D:961:U:C5	2.47	0.49
1:D:969:G:C6	1:D:970:G:N7	2.80	0.49
2:A:100:GLN:HB3	2:A:107:ILE:HD11	1.94	0.49
2:A:401:HIS:HD2	2:A:426:PHE:CD1	2.29	0.49
2:B:45:MET:HE3	2:B:48:GLU:HG2	1.93	0.49
2:B:165:ASN:OD1	2:B:191:ILE:HG21	2.12	0.49
2:B:563:GLY:C	2:B:565:GLU:N	2.69	0.49
2:A:9:LYS:HE2	2:A:571:TYR:CE2	2.47	0.49
2:A:260:ASP:OD1	2:A:300:ARG:CD	2.60	0.49
2:A:437:ILE:HG23	2:A:438:LYS:H	1.74	0.49
2:B:9:LYS:HA	2:B:571:TYR:CE1	2.47	0.49
2:B:45:MET:CE	2:B:48:GLU:HG2	2.41	0.49
2:B:67:ILE:HG22	2:B:68:TYR:N	2.27	0.49
2:B:108:GLU:O	2:B:109:VAL:HB	2.13	0.49
2:B:308:ASN:O	2:B:312:ILE:HG13	2.12	0.49
2:B:538:ILE:HD11	2:B:544:VAL:HG11	1.93	0.49
2:B:547:VAL:CG1	2:B:548:ASN:N	2.74	0.49
1:C:934:U:H5'	1:C:935:U:OP2	2.12	0.49
1:C:960:G:H2'	1:C:961:U:C5'	2.39	0.49
2:A:128:PHE:CD1	2:A:128:PHE:C	2.90	0.49
2:A:414:THR:HG21	2:A:443:ILE:HG12	1.94	0.49
2:A:435:ASP:O	2:A:436:ALA:C	2.55	0.49
2:A:151:SER:HA	2:A:154:ARG:CZ	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:473:LYS:HB3	2:A:478:ARG:HA	1.94	0.49
2:A:214:ILE:O	2:A:215:SER:C	2.55	0.49
2:B:350:LEU:HD11	2:B:378:TRP:HA	1.94	0.49
2:A:37:MET:HG2	2:A:59:ILE:HG12	1.94	0.49
2:A:181:ALA:HB1	2:A:220:LEU:CD2	2.39	0.49
2:B:13:LYS:HD3	2:B:23:LYS:HG3	1.95	0.49
2:B:64:SER:O	2:B:67:ILE:HB	2.11	0.49
2:B:154:ARG:HH12	2:B:183:ARG:HE	1.59	0.49
2:B:500:HIS:C	2:B:500:HIS:HD1	2.20	0.49
2:A:179:TYR:C	2:A:181:ALA:N	2.70	0.49
2:B:38:PRO:HG2	2:B:57:PHE:CD1	2.47	0.49
2:B:65:TYR:HB2	2:B:96:SER:O	2.13	0.49
2:B:139:ARG:HH21	2:B:176:LEU:HD21	1.77	0.49
2:B:329:TRP:CZ2	2:B:356:LEU:HD13	2.48	0.49
2:A:178:ARG:O	2:A:181:ALA:HB3	2.13	0.48
2:B:458:ASP:O	2:B:474:VAL:HG12	2.13	0.48
2:A:37:MET:O	2:A:249:ASP:HA	2.12	0.48
2:A:287:TYR:CD2	2:A:292:LEU:HB2	2.48	0.48
2:A:513:ASN:ND2	2:A:515:GLU:H	2.10	0.48
2:B:37:MET:HG2	2:B:248:PHE:O	2.12	0.48
2:B:135:PRO:CG	2:B:200:LEU:HD13	2.43	0.48
2:B:360:GLU:HB3	2:B:383:ARG:NH2	2.28	0.48
2:B:435:ASP:O	2:B:436:ALA:C	2.56	0.48
2:B:547:VAL:HG13	2:B:552:GLU:N	2.27	0.48
1:C:926:C:O2'	2:A:466:THR:O	2.31	0.48
1:C:957:C:N4	1:C:958:A:C6	2.81	0.48
2:A:114:ILE:CD1	2:A:129:LEU:HB2	2.43	0.48
2:A:227:HIS:HD1	2:A:228:LEU:N	2.11	0.48
2:A:281:CYS:HB2	2:A:282:PRO:CD	2.42	0.48
2:A:381:VAL:HG13	2:A:404:PHE:HE2	1.79	0.48
2:B:131:ILE:HG22	2:B:149:THR:OG1	2.12	0.48
2:B:401:HIS:HE1	2:B:403:ILE:HD13	1.79	0.48
2:B:533:PHE:HA	2:B:567:ILE:CG1	2.43	0.48
2:A:563:GLY:C	2:A:565:GLU:N	2.70	0.48
2:B:185:SER:HB3	2:B:221:ARG:HE	1.76	0.48
2:B:250:SER:CB	2:B:252:SER:OG	2.58	0.48
2:B:256:TYR:O	2:B:257:ALA:C	2.56	0.48
2:B:415:TYR:CE2	2:B:416:PRO:HB3	2.47	0.48
2:B:497:LYS:HD3	2:B:553:LEU:HB3	1.96	0.48
2:A:82:ILE:CD1	2:A:83:HIS:N	2.73	0.48
2:A:391:ILE:H	2:A:391:ILE:CD1	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:519:PHE:O	2:B:522:LYS:N	2.46	0.48
1:C:913:U:O2'	1:C:914:A:P	2.71	0.48
2:A:36:ILE:HG21	2:A:312:ILE:CG2	2.43	0.48
2:A:51:GLU:O	2:A:52:LEU:C	2.54	0.48
2:A:261:ARG:HG2	2:A:270:ARG:HD2	1.96	0.48
2:A:262:TYR:CE1	2:A:307:HIS:CE1	3.02	0.48
2:A:321:GLN:NE2	2:B:274:LEU:HA	2.28	0.48
2:A:521:ARG:HD3	2:A:582:GLU:OE1	2.13	0.48
2:B:37:MET:HG3	2:B:249:ASP:CB	2.44	0.48
2:B:396:GLY:O	2:B:408:SER:CB	2.61	0.48
2:B:486:ASP:C	2:B:486:ASP:OD2	2.55	0.48
2:B:491:LEU:HD11	2:B:499:LEU:HD22	1.95	0.48
2:B:517:GLU:N	2:B:518:PRO:CD	2.76	0.48
1:D:961:U:O2'	1:D:962:C:OP1	2.26	0.48
2:A:548:ASN:CA	2:A:554:LEU:HD11	2.43	0.48
2:B:204:TYR:CD1	2:B:206:PHE:CE1	3.01	0.48
1:C:959:A:O2'	1:C:960:G:O5'	2.31	0.48
1:D:915:G:H5''	2:A:230:GLY:HA2	1.95	0.48
2:A:44:GLN:O	2:A:44:GLN:HG3	2.14	0.48
2:B:128:PHE:HE2	2:B:166:ALA:HA	1.77	0.48
2:B:179:TYR:C	2:B:181:ALA:N	2.70	0.48
2:B:454:ARG:HB2	2:B:502:VAL:HG21	1.96	0.48
2:B:570:GLN:HE21	2:B:570:GLN:CA	2.26	0.48
2:A:49:PRO:O	2:A:50:LYS:C	2.57	0.48
2:A:65:TYR:CE2	2:A:107:ILE:HG13	2.48	0.48
2:A:132:PRO:HA	2:A:169:GLN:CD	2.39	0.48
2:A:206:PHE:CE1	2:A:236:VAL:HG13	2.48	0.48
1:C:917:U:H4'	2:B:66:ILE:CD1	2.44	0.48
2:A:65:TYR:CZ	2:A:107:ILE:HG13	2.49	0.48
2:A:165:ASN:HD22	2:A:191:ILE:HB	1.79	0.48
2:A:313:LYS:O	2:A:316:ILE:HG22	2.14	0.48
2:A:340:PRO:HB3	2:B:422:ALA:HA	1.96	0.48
2:B:111:ASN:O	2:B:115:ILE:HB	2.13	0.48
2:B:507:ARG:O	2:B:508:MET:CG	2.62	0.48
1:D:908:U:O2'	1:D:909:G:H5'	2.14	0.47
2:A:94:VAL:O	2:A:127:THR:OG1	2.32	0.47
2:A:140:GLU:HA	2:A:143:VAL:CG2	2.44	0.47
2:A:140:GLU:HB2	2:A:144:LYS:HE2	1.96	0.47
2:A:477:LYS:HZ2	2:A:478:ARG:N	1.90	0.47
2:B:395:PHE:N	2:B:395:PHE:CD1	2.81	0.47
2:B:416:PRO:HD2	2:B:417:PHE:CD1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:578:ARG:HH11	2:B:578:ARG:CG	2.26	0.47
2:A:68:TYR:HD1	2:A:117:PHE:CD2	2.31	0.47
2:A:179:TYR:C	2:A:181:ALA:H	2.22	0.47
2:A:343:TYR:CZ	2:A:347:LYS:HD3	2.48	0.47
2:A:456:PHE:O	2:A:457:ASP:C	2.56	0.47
2:B:36:ILE:CG2	2:B:316:ILE:HD11	2.43	0.47
2:B:163:PRO:HB3	2:B:190:GLU:HG3	1.95	0.47
2:B:401:HIS:CE1	2:B:403:ILE:HD13	2.49	0.47
2:B:548:ASN:OD1	2:B:552:GLU:HB2	2.15	0.47
2:B:563:GLY:C	2:B:565:GLU:H	2.22	0.47
2:A:311:VAL:O	2:A:312:ILE:C	2.58	0.47
2:A:511:VAL:HG12	2:A:547:VAL:HG23	1.95	0.47
2:B:397:GLU:HB2	2:B:410:TYR:HE1	1.80	0.47
1:D:905:C:N3	1:D:906:C:C5	2.83	0.47
1:D:976:C:N1	2:B:527:PHE:HD2	2.12	0.47
2:A:159:ILE:O	2:A:159:ILE:CG1	2.62	0.47
2:A:339:HIS:HD2	2:A:341:LYS:N	2.11	0.47
2:B:75:ARG:C	2:B:77:ALA:N	2.71	0.47
2:B:132:PRO:HA	2:B:169:GLN:CD	2.39	0.47
2:B:538:ILE:HG22	2:B:562:SER:C	2.38	0.47
2:A:9:LYS:HE2	2:A:571:TYR:CD2	2.50	0.47
2:A:253:TYR:CG	2:A:254:ALA:N	2.82	0.47
2:B:398:LEU:HD23	2:B:408:SER:N	2.29	0.47
2:B:469:PRO:O	2:B:482:VAL:HB	2.14	0.47
2:B:478:ARG:H	2:B:478:ARG:NE	2.12	0.47
2:B:561:LEU:CD1	2:B:569:PHE:CD1	2.95	0.47
2:A:75:ARG:C	2:A:77:ALA:N	2.71	0.47
2:A:327:GLU:O	2:A:328:LEU:C	2.57	0.47
2:A:451:GLY:O	2:A:453:SER:N	2.48	0.47
2:B:70:ASP:CB	2:B:73:LEU:HD12	2.44	0.47
2:B:85:MET:O	2:B:85:MET:HG2	2.14	0.47
2:B:136:ASP:H	2:B:172:THR:HG1	1.58	0.47
1:C:951:G:H2'	1:C:952:G:C8	2.49	0.47
2:A:214:ILE:HG22	2:A:215:SER:N	2.30	0.47
2:A:286:LYS:NZ	2:A:287:TYR:CE1	2.83	0.47
2:A:401:HIS:CE1	2:A:403:ILE:HB	2.50	0.47
2:A:463:LEU:HD23	2:A:469:PRO:HA	1.97	0.47
2:A:505:TYR:HA	2:A:509:ARG:HE	1.79	0.47
2:B:40:VAL:HG22	2:B:61:ILE:O	2.14	0.47
2:B:348:ARG:HA	2:B:351:GLU:HG3	1.97	0.47
2:B:415:TYR:HB2	2:B:419:GLN:HE21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:474:VAL:CG1	2:B:479:LEU:HD21	2.34	0.47
2:B:511:VAL:HB	2:B:533:PHE:O	2.14	0.47
2:B:461:VAL:HG22	2:B:472:VAL:HG12	1.97	0.47
2:A:98:SER:HB2	2:A:130:ASP:O	2.15	0.47
2:B:14:ALA:HB3	2:B:21:ILE:HG13	1.96	0.47
2:B:63:ASN:ND2	2:B:66:ILE:N	2.58	0.47
2:B:559:ALA:C	2:B:560:LEU:HD12	2.40	0.47
1:C:968:G:H5'	2:A:478:ARG:NH1	2.29	0.46
2:A:336:ALA:HA	2:A:342:LEU:HD22	1.93	0.46
2:B:330:ARG:HH12	2:B:331:LEU:HA	1.80	0.46
2:B:411:LEU:O	2:B:413:LEU:N	2.47	0.46
2:B:533:PHE:HA	2:B:567:ILE:HG13	1.96	0.46
2:A:38:PRO:CG	2:A:57:PHE:CD2	2.99	0.46
2:B:24:LEU:HB3	2:B:31:ILE:CG2	2.44	0.46
2:A:316:ILE:CG2	2:A:317:LYS:N	2.78	0.46
2:B:8:LEU:HD23	2:B:9:LYS:N	2.30	0.46
2:B:19:GLY:HA2	2:B:244:GLY:HA2	1.97	0.46
2:B:164:MET:H	2:B:190:GLU:CG	2.28	0.46
2:B:327:GLU:O	2:B:328:LEU:C	2.58	0.46
2:B:362:ILE:HD12	2:B:542:ASP:OD1	2.15	0.46
2:B:536:PRO:C	2:B:538:ILE:H	2.22	0.46
1:C:924:G:C6	1:C:925:A:C6	3.03	0.46
1:D:936:A:N1	1:D:937:C:C5	2.83	0.46
2:A:102:MET:HB2	2:A:132:PRO:HG2	1.97	0.46
2:A:398:LEU:HD23	2:A:398:LEU:N	2.29	0.46
2:A:413:LEU:HA	2:A:418:ALA:HB2	1.96	0.46
2:A:474:VAL:O	2:A:475:ASN:HB2	2.14	0.46
2:B:456:PHE:O	2:B:457:ASP:C	2.58	0.46
1:C:970:G:H2'	1:C:971:C:H6	1.81	0.46
1:D:967:C:C6	1:D:967:C:H3'	2.50	0.46
2:A:183:ARG:CZ	2:A:183:ARG:HA	2.45	0.46
2:A:394:ARG:HG3	2:A:394:ARG:HH11	1.81	0.46
2:A:415:TYR:HB2	2:A:486:ASP:HB2	1.98	0.46
2:B:10:PHE:CD2	2:B:225:PRO:HG3	2.49	0.46
2:B:328:LEU:O	2:B:332:VAL:HG23	2.15	0.46
1:C:913:U:O2'	1:C:914:A:O5'	2.33	0.46
2:A:277:PHE:HA	2:A:278:PRO:HD2	1.82	0.46
2:A:546:VAL:HB	2:A:555:ALA:O	2.16	0.46
2:B:178:ARG:HG2	2:B:219:ALA:HB2	1.96	0.46
1:D:915:G:H5''	2:A:230:GLY:HA3	1.98	0.46
2:A:24:LEU:HD23	2:A:31:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:39:VAL:HA	2:A:61:ILE:HG23	1.98	0.46
2:A:98:SER:CB	2:A:130:ASP:O	2.64	0.46
2:A:264:THR:C	2:A:266:GLU:N	2.72	0.46
2:B:128:PHE:CE2	2:B:166:ALA:HA	2.51	0.46
2:B:442:ALA:C	2:B:444:ALA:N	2.72	0.46
1:D:971:C:H2'	1:D:972:C:C6	2.51	0.46
2:A:85:MET:HE2	2:A:85:MET:O	2.16	0.46
2:A:154:ARG:HA	2:A:187:MET:CE	2.46	0.46
2:A:233:HIS:ND1	2:A:234:PRO:CD	2.76	0.46
2:A:262:TYR:CE1	2:A:307:HIS:NE2	2.84	0.46
2:A:403:ILE:HD12	2:A:420:SER:CB	2.46	0.46
2:A:454:ARG:C	2:A:456:PHE:N	2.74	0.46
2:A:548:ASN:HB3	2:A:554:LEU:HD21	1.96	0.46
1:D:957:C:H6	1:D:957:C:O5'	1.99	0.46
2:A:59:ILE:HG13	2:A:60:ILE:N	2.29	0.46
2:A:139:ARG:O	2:A:143:VAL:HG23	2.16	0.46
2:B:51:GLU:O	2:B:52:LEU:C	2.59	0.46
2:B:343:TYR:CE2	2:B:347:LYS:HE2	2.51	0.46
2:B:448:PHE:CA	2:B:508:MET:HE1	2.46	0.46
2:A:503:LEU:HA	2:A:504:PRO:HD2	1.75	0.46
2:A:533:PHE:HA	2:A:567:ILE:CG1	2.46	0.46
2:B:454:ARG:C	2:B:456:PHE:N	2.74	0.46
1:C:948:U:O2'	1:C:949:C:H5'	2.16	0.45
2:A:256:TYR:O	2:A:257:ALA:C	2.58	0.45
2:B:409:ARG:HA	2:B:412:SER:HB3	1.98	0.45
2:B:441:MET:HE2	2:B:453:SER:OG	2.15	0.45
2:B:554:LEU:O	2:B:555:ALA:HB2	2.16	0.45
1:C:916:U:C2'	1:C:917:U:OP1	2.64	0.45
2:A:157:GLU:O	2:A:160:LYS:HG2	2.15	0.45
2:A:187:MET:CB	2:A:189:PHE:CE1	2.92	0.45
2:A:511:VAL:HG22	2:A:533:PHE:C	2.36	0.45
2:B:131:ILE:O	2:B:131:ILE:HG23	2.14	0.45
1:D:931:C:O2'	1:D:932:C:H5'	2.15	0.45
2:A:187:MET:O	2:A:224:ARG:NH2	2.43	0.45
2:A:297:LYS:HZ3	2:A:301:THR:HG23	1.79	0.45
2:A:505:TYR:HA	2:A:509:ARG:NH2	2.29	0.45
2:A:84:ARG:HH22	2:A:87:ASP:HA	1.82	0.45
2:A:533:PHE:CD1	2:A:567:ILE:HD11	2.51	0.45
2:B:497:LYS:CD	2:B:553:LEU:HD23	2.46	0.45
2:B:545:LEU:N	2:B:545:LEU:HD23	2.32	0.45
2:B:568:VAL:HG12	2:B:568:VAL:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:912:C:O3'	2:B:204:TYR:CE2	2.69	0.45
2:A:82:ILE:O	2:A:83:HIS:C	2.59	0.45
2:B:45:MET:CE	2:B:48:GLU:HA	2.45	0.45
1:D:909:G:C5	2:B:428:ILE:CD1	2.99	0.45
2:A:237:PHE:N	2:A:237:PHE:HD2	2.14	0.45
2:A:348:ARG:O	2:A:351:GLU:HB2	2.17	0.45
2:A:540:PRO:C	2:A:541:TYR:CD1	2.94	0.45
2:B:8:LEU:C	2:B:8:LEU:CD2	2.87	0.45
2:B:183:ARG:O	2:B:187:MET:HG3	2.16	0.45
2:B:256:TYR:CD1	2:B:263:MET:HE2	2.51	0.45
2:B:358:GLU:O	2:B:539:ARG:CD	2.57	0.45
2:B:359:PHE:O	2:B:361:PRO:HD3	2.17	0.45
2:B:437:ILE:O	2:B:440:VAL:N	2.50	0.45
1:C:907:G:C4'	1:C:908:U:C6	2.99	0.45
2:B:206:PHE:O	2:B:210:VAL:HG23	2.16	0.45
2:B:415:TYR:C	2:B:415:TYR:CD2	2.94	0.45
2:B:491:LEU:HB2	2:B:556:THR:HG21	1.99	0.45
2:A:221:ARG:NH2	2:A:224:ARG:HD2	2.27	0.45
2:A:269:LYS:HB3	2:A:274:LEU:CD2	2.47	0.45
2:A:474:VAL:HG11	2:A:498:ARG:NH1	2.32	0.45
2:B:233:HIS:O	2:B:236:VAL:HG23	2.16	0.45
2:B:337:ARG:NH2	2:B:372:SER:HB2	2.32	0.45
2:B:455:ALA:HB2	2:B:502:VAL:CG1	2.47	0.45
2:B:493:ILE:HG23	2:B:494:GLU:H	1.80	0.45
2:A:29:LYS:O	2:A:91:ILE:HD11	2.16	0.45
2:A:99:PHE:CE1	2:A:198:VAL:HG21	2.47	0.45
2:A:264:THR:O	2:A:266:GLU:N	2.50	0.45
2:B:49:PRO:O	2:B:50:LYS:C	2.58	0.45
2:B:304:LEU:O	2:B:305:ALA:C	2.60	0.45
1:C:935:U:H2'	1:C:936:A:C4	2.52	0.45
1:C:939:A:O5'	1:C:939:A:H8	2.00	0.45
2:A:400:GLU:HA	2:A:405:GLY:O	2.17	0.45
2:B:339:HIS:HE1	2:B:341:LYS:HG2	1.81	0.45
2:A:37:MET:HE1	2:A:93:GLU:OE2	2.17	0.44
2:A:499:LEU:O	2:A:500:HIS:C	2.60	0.44
2:A:503:LEU:HA	2:A:503:LEU:HD23	1.80	0.44
2:A:554:LEU:O	2:A:555:ALA:HB2	2.17	0.44
2:B:162:ILE:HD12	2:B:163:PRO:CD	2.34	0.44
2:B:167:THR:HG1	2:B:193:PRO:HG2	1.82	0.44
2:B:339:HIS:CG	2:B:340:PRO:HD2	2.52	0.44
2:B:529:LYS:HG2	2:B:530:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:538:ILE:O	2:B:562:SER:HA	2.17	0.44
1:D:915:G:C2	2:A:229:PHE:CE1	3.05	0.44
2:A:75:ARG:O	2:A:76:LYS:C	2.60	0.44
2:B:37:MET:HB2	2:B:61:ILE:HG22	1.99	0.44
2:B:63:ASN:HB3	2:B:66:ILE:CG1	2.45	0.44
2:B:350:LEU:HD12	2:B:377:ARG:O	2.17	0.44
2:B:549:GLU:O	2:B:549:GLU:HG2	2.16	0.44
2:A:18:ALA:HB3	2:A:242:ALA:O	2.17	0.44
2:A:80:LEU:HD13	2:A:84:ARG:HD3	2.00	0.44
2:A:112:ARG:NH2	2:A:159:ILE:HD13	2.33	0.44
2:A:175:ASP:OD1	2:A:176:LEU:HG	2.17	0.44
2:A:356:LEU:H	2:A:356:LEU:HD22	1.82	0.44
2:A:566:MET:HE3	2:A:566:MET:HB2	1.91	0.44
2:B:330:ARG:NH1	2:B:330:ARG:C	2.76	0.44
2:B:448:PHE:HB2	2:B:452:ALA:CB	2.47	0.44
1:C:914:A:H2'	2:B:230:GLY:O	2.17	0.44
1:D:961:U:C2'	1:D:962:C:OP1	2.66	0.44
2:A:33:THR:HA	2:A:34:PRO:C	2.43	0.44
2:B:98:SER:O	2:B:101:LEU:N	2.50	0.44
2:B:98:SER:HA	2:B:101:LEU:HB3	1.99	0.44
1:C:957:C:H2'	1:C:958:A:C5'	2.34	0.44
2:A:36:ILE:HG13	2:A:248:PHE:CB	2.47	0.44
2:A:111:ASN:O	2:A:115:ILE:CG1	2.63	0.44
2:A:262:TYR:CD1	2:A:307:HIS:NE2	2.85	0.44
2:A:448:PHE:HB2	2:A:452:ALA:HB2	2.00	0.44
2:B:47:VAL:HG12	2:B:52:LEU:CD1	2.47	0.44
2:B:110:SER:O	2:B:111:ASN:C	2.60	0.44
2:B:179:TYR:C	2:B:181:ALA:H	2.24	0.44
1:C:908:U:OP1	2:A:465:LYS:HG2	2.18	0.44
2:A:9:LYS:HB3	2:A:25:GLU:HB3	1.99	0.44
2:A:137:ALA:HB1	2:A:141:GLN:HE22	1.83	0.44
2:A:227:HIS:ND1	2:A:247:LEU:O	2.50	0.44
2:A:249:ASP:O	2:A:250:SER:HB3	2.17	0.44
2:A:290:GLN:HA	2:A:293:ARG:CD	2.47	0.44
2:B:130:ASP:OD2	2:B:167:THR:CB	2.64	0.44
2:B:525:ASP:OD1	2:B:577:VAL:N	2.51	0.44
1:D:959:A:H4'	1:D:960:G:OP1	2.18	0.44
2:A:362:ILE:HD12	2:A:362:ILE:HA	1.87	0.44
2:B:221:ARG:HB3	2:B:223:ASP:OD1	2.17	0.44
2:B:322:ALA:CB	2:B:328:LEU:HD22	2.48	0.44
2:B:496:ALA:CB	2:B:556:THR:OG1	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:499:LEU:O	2:B:502:VAL:N	2.48	0.44
2:A:73:LEU:O	2:A:74:ARG:C	2.61	0.44
2:B:120:ARG:C	2:B:122:GLY:H	2.25	0.44
2:B:413:LEU:HD21	2:B:429:GLU:O	2.18	0.44
2:B:419:GLN:OE1	2:B:419:GLN:N	2.51	0.44
2:B:503:LEU:CD2	2:B:508:MET:SD	3.06	0.44
1:C:967:C:H2'	2:A:471:GLN:HE22	1.82	0.44
2:A:460:LYS:O	2:A:472:VAL:HA	2.17	0.44
2:A:527:PHE:O	2:A:528:ALA:C	2.60	0.44
2:B:174:THR:OG1	2:B:215:SER:HB2	2.17	0.44
1:C:916:U:H2'	1:C:916:U:O2	2.18	0.43
2:A:83:HIS:HE1	2:A:124:ASP:OD2	2.00	0.43
2:A:239:LEU:C	2:A:239:LEU:CD2	2.90	0.43
2:A:252:SER:OG	2:A:253:TYR:N	2.50	0.43
2:A:316:ILE:HG22	2:A:317:LYS:N	2.33	0.43
2:A:382:ARG:HG3	2:A:382:ARG:HH11	1.83	0.43
2:A:411:LEU:O	2:A:413:LEU:N	2.51	0.43
2:A:525:ASP:OD1	2:A:576:LYS:HA	2.18	0.43
2:A:527:PHE:O	2:A:529:LYS:N	2.51	0.43
2:B:560:LEU:O	2:B:561:LEU:HD23	2.17	0.43
1:C:913:U:O3'	2:B:256:TYR:CE2	2.71	0.43
1:D:909:G:N2	1:D:910:G:H1'	2.34	0.43
1:D:916:U:OP1	2:A:99:PHE:CB	2.65	0.43
2:A:20:ARG:NH2	2:A:217:LYS:NZ	2.66	0.43
2:A:38:PRO:HD3	2:A:57:PHE:CD2	2.52	0.43
2:A:175:ASP:OD1	2:A:176:LEU:N	2.51	0.43
2:A:493:ILE:O	2:A:496:ALA:HB3	2.18	0.43
2:B:52:LEU:HD12	2:B:52:LEU:H	1.83	0.43
2:B:178:ARG:NH1	2:B:178:ARG:CB	2.81	0.43
2:B:436:ALA:HB1	2:B:461:VAL:HB	1.99	0.43
2:B:499:LEU:O	2:B:500:HIS:C	2.61	0.43
1:C:946:G:H2'	1:C:947:G:OP2	2.18	0.43
1:D:940:G:H21	2:A:136:ASP:HB3	1.83	0.43
2:A:149:THR:H	2:A:149:THR:HG1	1.60	0.43
2:A:264:THR:O	2:A:265:PRO:C	2.61	0.43
2:A:371:ILE:C	2:A:371:ILE:HD12	2.43	0.43
2:A:372:SER:O	2:A:375:SER:HB3	2.18	0.43
2:A:432:THR:O	2:A:433:LYS:C	2.61	0.43
2:B:51:GLU:O	2:B:54:LYS:N	2.50	0.43
2:B:147:GLU:OE2	2:B:179:TYR:OH	2.33	0.43
2:B:396:GLY:O	2:B:397:GLU:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:912:C:H2'	1:D:913:U:C6	2.53	0.43
1:D:933:C:H1'	2:A:136:ASP:HB3	2.01	0.43
2:A:154:ARG:HA	2:A:187:MET:HE1	2.00	0.43
2:A:246:ASP:O	2:A:247:LEU:HD23	2.18	0.43
2:A:560:LEU:HD11	2:A:576:LYS:CD	2.48	0.43
2:B:37:MET:HG3	2:B:249:ASP:HB2	2.00	0.43
2:B:48:GLU:O	2:B:52:LEU:HD12	2.18	0.43
2:B:431:PRO:HG3	2:B:469:PRO:CG	2.48	0.43
1:C:914:A:H5''	2:B:202:GLU:OE2	2.18	0.43
1:D:948:U:H2'	1:D:949:C:O4'	2.18	0.43
2:A:38:PRO:HD3	2:A:57:PHE:HD2	1.82	0.43
2:A:200:LEU:HD23	2:A:200:LEU:HA	1.82	0.43
2:A:394:ARG:HG3	2:A:394:ARG:NH1	2.33	0.43
2:A:497:LYS:HA	2:A:553:LEU:HD22	2.01	0.43
1:C:968:G:O4'	2:A:471:GLN:NE2	2.52	0.43
1:D:949:C:N4	1:D:960:G:H21	2.16	0.43
2:A:321:GLN:NE2	2:B:275:ASP:N	2.51	0.43
2:B:511:VAL:HG12	2:B:532:ILE:CG2	2.49	0.43
1:D:974:A:C6	1:D:975:C:N4	2.87	0.43
2:A:37:MET:HG2	2:A:59:ILE:CG1	2.48	0.43
2:A:214:ILE:HD13	2:A:214:ILE:HA	1.78	0.43
2:A:286:LYS:NZ	2:A:287:TYR:HE1	2.16	0.43
2:A:395:PHE:CD1	2:A:395:PHE:N	2.86	0.43
2:A:578:ARG:HG2	2:A:578:ARG:HH11	1.84	0.43
1:C:962:C:H2'	1:C:963:C:H6	1.79	0.43
2:A:61:ILE:HG12	2:A:62:THR:N	2.29	0.43
2:A:411:LEU:HD23	2:A:411:LEU:HA	1.86	0.43
2:A:515:GLU:O	2:A:518:PRO:HD2	2.18	0.43
2:A:529:LYS:HG3	2:A:570:GLN:O	2.19	0.43
2:B:12:ILE:HG13	2:B:20:ARG:HG3	2.01	0.43
2:B:348:ARG:O	2:B:349:LEU:C	2.58	0.43
2:B:495:GLY:O	2:B:498:ARG:HB2	2.19	0.43
2:B:515:GLU:O	2:B:518:PRO:HD2	2.17	0.43
1:D:960:G:N3	1:D:960:G:H5'	2.34	0.43
2:A:290:GLN:HA	2:A:293:ARG:HD2	2.00	0.43
2:B:251:ALA:HB3	2:B:255:LEU:HD12	1.99	0.43
1:C:909:G:N2	1:C:910:G:H1'	2.34	0.43
1:C:918:G:H2'	1:C:918:G:N3	2.32	0.43
1:D:914:A:H1'	2:A:252:SER:CB	2.45	0.43
2:A:98:SER:HB2	2:A:132:PRO:CD	2.49	0.43
2:A:303:LEU:HD23	2:A:306:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:449:GLY:O	2:A:450:GLU:C	2.62	0.43
2:A:567:ILE:HG22	2:A:568:VAL:HG12	2.01	0.43
2:B:224:ARG:HA	2:B:225:PRO:HD3	1.91	0.43
2:B:264:THR:C	2:B:266:GLU:N	2.77	0.43
2:B:321:GLN:O	2:B:325:GLU:HG2	2.19	0.43
2:B:335:ARG:HG2	2:B:335:ARG:NH1	2.32	0.43
2:B:538:ILE:HG22	2:B:538:ILE:O	2.19	0.43
2:A:131:ILE:HD13	2:A:131:ILE:N	2.33	0.42
2:A:290:GLN:C	2:A:293:ARG:HG2	2.41	0.42
2:A:342:LEU:C	2:A:342:LEU:HD23	2.44	0.42
2:A:435:ASP:C	2:A:437:ILE:N	2.76	0.42
2:B:178:ARG:HB2	2:B:178:ARG:CZ	2.49	0.42
2:B:272:ASP:HA	2:B:293:ARG:HE	1.84	0.42
2:B:333:ASP:OD2	2:B:337:ARG:NH2	2.45	0.42
2:B:337:ARG:NH2	2:B:372:SER:CB	2.82	0.42
2:B:448:PHE:HB2	2:B:452:ALA:HB2	2.00	0.42
2:B:529:LYS:HG2	2:B:530:PHE:CE2	2.53	0.42
1:D:953:G:C2	1:D:964:C:N3	2.87	0.42
2:A:12:ILE:HG12	2:A:20:ARG:HG3	2.00	0.42
2:A:357:GLU:OE1	2:A:383:ARG:HD3	2.19	0.42
2:A:488:LEU:HD23	2:A:488:LEU:HA	1.60	0.42
2:B:268:THR:C	2:B:269:LYS:HD3	2.43	0.42
2:B:283:VAL:HG13	2:B:303:LEU:HD22	2.01	0.42
2:B:443:ILE:HG22	2:B:489:LEU:HD22	2.00	0.42
2:A:423:GLU:CD	2:A:423:GLU:H	2.25	0.42
2:A:448:PHE:HB2	2:A:452:ALA:CB	2.49	0.42
2:A:563:GLY:O	2:A:564:ARG:C	2.63	0.42
2:B:31:ILE:HD12	2:B:59:ILE:CG2	2.50	0.42
2:B:37:MET:O	2:B:249:ASP:HA	2.19	0.42
2:B:265:PRO:CB	2:B:335:ARG:HE	2.26	0.42
1:C:968:G:H4'	2:A:471:GLN:HE21	1.84	0.42
1:D:906:C:O2'	1:D:907:G:H5'	2.19	0.42
2:A:261:ARG:CG	2:A:270:ARG:HH11	2.32	0.42
2:A:266:GLU:HG2	2:B:330:ARG:NH2	2.33	0.42
2:A:468:MET:HA	2:A:469:PRO:HD3	1.83	0.42
2:A:536:PRO:C	2:A:538:ILE:H	2.27	0.42
2:B:322:ALA:HA	2:B:327:GLU:HG2	2.02	0.42
2:B:346:TYR:CE2	2:B:374:GLU:HG2	2.54	0.42
2:B:432:THR:O	2:B:433:LYS:C	2.61	0.42
2:B:527:PHE:O	2:B:528:ALA:C	2.63	0.42
2:B:563:GLY:O	2:B:564:ARG:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:970:G:O2'	1:C:971:C:H5'	2.19	0.42
1:D:901:G:O5'	1:D:901:G:H8	2.02	0.42
1:D:938:G:O2'	2:B:425:ASP:HB2	2.19	0.42
2:A:18:ALA:HB2	2:A:356:LEU:HD12	2.02	0.42
2:A:213:VAL:HB	2:A:243:MET:CE	2.49	0.42
2:B:497:LYS:HD3	2:B:553:LEU:CB	2.50	0.42
1:C:913:U:O3'	2:B:256:TYR:HE2	2.02	0.42
2:A:83:HIS:CE1	2:A:124:ASP:OD2	2.73	0.42
2:B:286:LYS:C	2:B:287:TYR:CD1	2.98	0.42
2:B:325:GLU:O	2:B:366:SER:OG	2.35	0.42
2:B:409:ARG:O	2:B:412:SER:N	2.52	0.42
2:A:67:ILE:O	2:A:74:ARG:HG2	2.19	0.42
2:A:80:LEU:HD23	2:A:80:LEU:HA	1.91	0.42
2:A:147:GLU:O	2:A:148:ILE:C	2.63	0.42
2:A:359:PHE:H	2:A:359:PHE:HD1	1.67	0.42
2:B:402:PRO:HB2	2:B:403:ILE:HD12	2.02	0.42
2:B:409:ARG:O	2:B:412:SER:HB3	2.19	0.42
1:C:913:U:H5''	2:B:256:TYR:OH	2.20	0.42
2:A:261:ARG:HG3	2:A:270:ARG:NH1	2.34	0.42
2:A:396:GLY:O	2:A:397:GLU:C	2.63	0.42
2:B:322:ALA:HB3	2:B:328:LEU:HD22	2.01	0.42
2:B:328:LEU:HD22	2:B:328:LEU:HA	1.68	0.42
2:B:410:TYR:CE2	2:B:438:LYS:HD3	2.54	0.42
2:B:435:ASP:O	2:B:438:LYS:N	2.53	0.42
2:B:508:MET:HE2	2:B:508:MET:HB3	1.74	0.42
2:B:514:LYS:HG3	2:B:515:GLU:N	2.35	0.42
2:A:110:SER:O	2:A:111:ASN:C	2.63	0.42
2:A:503:LEU:O	2:A:509:ARG:NH2	2.45	0.42
2:B:175:ASP:HA	2:B:178:ARG:HH12	1.84	0.42
2:B:264:THR:O	2:B:266:GLU:N	2.52	0.42
2:B:290:GLN:CG	2:B:291:GLU:N	2.63	0.42
2:B:318:ARG:HH11	2:B:318:ARG:HB3	1.84	0.42
2:B:329:TRP:HB3	2:B:378:TRP:CE2	2.55	0.42
2:A:82:ILE:HD12	2:A:83:HIS:ND1	2.35	0.42
2:A:184:LEU:C	2:A:192:HIS:HE2	2.28	0.42
2:A:234:PRO:HB2	2:A:265:PRO:HA	2.02	0.42
2:A:249:ASP:O	2:A:249:ASP:CG	2.61	0.42
2:A:415:TYR:HA	2:A:419:GLN:OE1	2.19	0.42
2:A:432:THR:HB	2:A:433:LYS:CE	2.44	0.42
2:A:433:LYS:HG2	2:A:434:GLU:OE2	2.19	0.42
2:B:82:ILE:O	2:B:83:HIS:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:401:HIS:CD2	2:B:404:PHE:HD1	2.38	0.42
2:A:178:ARG:HH21	2:A:218:MET:HE1	1.84	0.41
2:A:245:VAL:CG1	2:A:246:ASP:N	2.82	0.41
2:A:554:LEU:O	2:A:581:VAL:HG12	2.19	0.41
2:B:131:ILE:O	2:B:169:GLN:HG3	2.20	0.41
2:B:449:GLY:O	2:B:451:GLY:N	2.53	0.41
2:B:470:ARG:HA	2:B:482:VAL:HB	2.02	0.41
1:C:948:U:H6	1:C:948:U:O5'	2.02	0.41
1:C:969:G:C2	1:C:970:G:C8	3.08	0.41
1:D:914:A:O2'	1:D:915:G:P	2.78	0.41
1:D:947:G:H5'	1:D:948:U:OP2	2.20	0.41
2:A:207:ARG:HD2	2:A:348:ARG:HH12	1.81	0.41
2:A:560:LEU:HD11	2:A:576:LYS:HG3	2.02	0.41
2:B:31:ILE:HD12	2:B:59:ILE:HG21	1.99	0.41
2:B:462:GLU:OE2	2:B:471:GLN:HB2	2.20	0.41
1:D:901:G:N2	1:D:973:C:O2	2.52	0.41
1:D:936:A:N6	1:D:937:C:N3	2.68	0.41
1:D:967:C:C6	1:D:967:C:C3'	3.03	0.41
2:A:470:ARG:NH1	2:A:484:ALA:CA	2.70	0.41
2:B:62:THR:O	2:B:94:VAL:HG12	2.20	0.41
2:B:386:GLU:O	2:B:389:LYS:HB2	2.20	0.41
2:B:392:ASN:ND2	2:B:408:SER:H	2.18	0.41
1:C:946:G:O2'	1:C:947:G:H8	2.02	0.41
2:A:348:ARG:O	2:A:349:LEU:C	2.62	0.41
2:A:560:LEU:HD11	2:A:576:LYS:HD2	2.02	0.41
2:B:323:ILE:HG12	2:B:328:LEU:HD23	2.01	0.41
1:C:916:U:C6	2:B:251:ALA:HB1	2.56	0.41
1:D:931:C:C2'	1:D:932:C:H5'	2.50	0.41
2:A:478:ARG:O	2:A:478:ARG:HG3	2.21	0.41
2:A:541:TYR:HA	2:A:558:GLN:HG3	2.01	0.41
2:A:563:GLY:C	2:A:565:GLU:H	2.28	0.41
2:B:181:ALA:HB3	2:B:219:ALA:HB3	2.03	0.41
2:B:538:ILE:CG2	2:B:563:GLY:N	2.74	0.41
2:B:548:ASN:O	2:B:550:ASN:N	2.54	0.41
2:A:80:LEU:HD13	2:A:84:ARG:HB3	2.02	0.41
2:A:245:VAL:HG12	2:A:246:ASP:N	2.34	0.41
2:A:437:ILE:CG2	2:A:438:LYS:H	2.33	0.41
2:B:327:GLU:O	2:B:327:GLU:HG3	2.20	0.41
1:C:936:A:C2	1:C:937:C:C5	3.08	0.41
1:C:941:G:C6	1:C:942:C:C4	3.09	0.41
1:D:905:C:C2	1:D:906:C:C6	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:962:C:C2	1:D:963:C:C4	3.09	0.41
2:A:109:VAL:HG22	2:A:110:SER:N	2.35	0.41
2:A:150:LEU:HD23	2:A:184:LEU:HD21	2.01	0.41
2:A:216:SER:O	2:A:217:LYS:C	2.63	0.41
2:A:266:GLU:OE1	2:B:334:GLU:OE2	2.38	0.41
2:A:370:LYS:HA	2:A:375:SER:OG	2.21	0.41
2:A:514:LYS:O	2:A:518:PRO:HD3	2.20	0.41
2:B:75:ARG:O	2:B:76:LYS:C	2.62	0.41
1:D:904:C:O2'	1:D:905:C:H5'	2.21	0.41
1:D:967:C:H4'	2:B:478:ARG:NH1	2.36	0.41
2:B:460:LYS:NZ	2:B:475:ASN:N	2.67	0.41
1:C:903:G:C2	1:C:972:C:C2	3.08	0.41
1:D:934:U:C4	1:D:936:A:H5'	2.55	0.41
2:A:29:LYS:HB2	2:A:91:ILE:HG12	2.03	0.41
2:A:183:ARG:HA	2:A:183:ARG:NE	2.36	0.41
2:A:183:ARG:HH11	2:A:183:ARG:HG2	1.86	0.41
2:A:257:ALA:O	2:A:301:THR:HG22	2.20	0.41
2:A:314:GLU:OE1	2:B:279:CYS:HA	2.20	0.41
2:A:357:GLU:OE1	2:A:383:ARG:CD	2.68	0.41
2:A:464:SER:C	2:A:466:THR:H	2.29	0.41
2:A:503:LEU:HD21	2:A:507:ARG:NH2	2.36	0.41
2:A:581:VAL:O	2:A:581:VAL:HG22	2.20	0.41
2:B:82:ILE:CG2	2:B:83:HIS:H	2.31	0.41
2:B:83:HIS:H	2:B:83:HIS:HD1	1.69	0.41
2:B:258:LYS:HA	2:B:301:THR:HG23	2.01	0.41
2:B:339:HIS:HA	2:B:340:PRO:HD3	1.91	0.41
2:B:455:ALA:HB3	2:B:499:LEU:HD12	2.03	0.41
2:B:464:SER:C	2:B:466:THR:H	2.28	0.41
2:B:511:VAL:HG11	2:B:532:ILE:HG22	2.03	0.41
2:B:514:LYS:O	2:B:518:PRO:HD3	2.21	0.41
2:A:413:LEU:N	2:A:413:LEU:CD1	2.61	0.41
2:A:470:ARG:HD3	2:A:470:ARG:HA	1.88	0.41
2:A:474:VAL:O	2:A:474:VAL:HG13	2.21	0.41
2:B:48:GLU:HB2	2:B:51:GLU:OE1	2.21	0.41
2:B:135:PRO:CG	2:B:200:LEU:CD1	2.98	0.41
2:B:544:VAL:C	2:B:545:LEU:HD23	2.46	0.41
1:C:973:C:H2'	1:C:974:A:C8	2.56	0.40
1:D:914:A:H3'	2:A:198:VAL:HG12	2.03	0.40
2:A:63:ASN:HB3	2:A:66:ILE:HD12	2.02	0.40
2:A:393:GLU:O	2:A:394:ARG:C	2.65	0.40
2:A:564:ARG:HE	2:A:564:ARG:HB3	1.43	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:VAL:HG12	2:B:52:LEU:HD12	2.03	0.40
2:B:73:LEU:O	2:B:74:ARG:C	2.63	0.40
2:B:435:ASP:C	2:B:437:ILE:N	2.79	0.40
2:B:480:ALA:HB1	2:B:490:THR:O	2.21	0.40
2:B:507:ARG:C	2:B:508:MET:CG	2.94	0.40
2:A:283:VAL:O	2:A:287:TYR:HB2	2.21	0.40
2:A:401:HIS:HE1	2:A:403:ILE:HB	1.86	0.40
2:B:203:SER:O	2:B:204:TYR:C	2.64	0.40
2:B:297:LYS:O	2:B:300:ARG:N	2.54	0.40
2:B:451:GLY:O	2:B:453:SER:N	2.54	0.40
1:D:914:A:H2'	2:A:230:GLY:O	2.21	0.40
2:A:85:MET:HE3	2:A:85:MET:HB2	1.89	0.40
2:A:499:LEU:O	2:A:502:VAL:N	2.54	0.40
2:B:167:THR:O	2:B:167:THR:HG22	2.21	0.40
2:B:233:HIS:HA	2:B:234:PRO:HD3	1.89	0.40
2:A:140:GLU:CA	2:A:143:VAL:HG23	2.50	0.40
2:B:120:ARG:C	2:B:122:GLY:N	2.80	0.40
2:B:492:GLY:O	2:B:493:ILE:C	2.64	0.40
2:B:499:LEU:O	2:B:501:ARG:N	2.55	0.40
2:A:85:MET:O	2:A:85:MET:CE	2.70	0.40
2:A:120:ARG:C	2:A:122:GLY:H	2.29	0.40
2:A:356:LEU:HD22	2:A:356:LEU:N	2.37	0.40
2:A:371:ILE:C	2:A:371:ILE:CD1	2.95	0.40
2:A:538:ILE:O	2:A:562:SER:HA	2.20	0.40
2:B:44:GLN:HE21	2:B:44:GLN:HB3	1.57	0.40
2:B:109:VAL:HG21	2:B:114:ILE:HB	2.03	0.40
2:B:223:ASP:HB3	2:B:569:PHE:CD2	2.56	0.40
2:B:330:ARG:HH11	2:B:330:ARG:CB	2.29	0.40
2:B:423:GLU:H	2:B:423:GLU:CD	2.29	0.40
2:B:456:PHE:N	2:B:456:PHE:CD1	2.90	0.40
2:B:458:ASP:O	2:B:474:VAL:CG1	2.69	0.40
2:B:485:ASP:OD1	2:B:486:ASP:N	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	574/582 (99%)	467 (81%)	86 (15%)	21 (4%)	2	17
2	B	574/582 (99%)	472 (82%)	78 (14%)	24 (4%)	2	14
All	All	1148/1164 (99%)	939 (82%)	164 (14%)	45 (4%)	2	16

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	412	SER
2	A	433	LYS
2	A	452	ALA
2	A	493	ILE
2	A	528	ALA
2	B	412	SER
2	B	433	LYS
2	B	436	ALA
2	B	452	ALA
2	B	493	ILE
2	A	109	VAL
2	A	436	ALA
2	A	564	ARG
2	B	109	VAL
2	B	423	GLU
2	B	528	ALA
2	B	549	GLU
2	A	297	LYS
2	A	423	GLU
2	A	457	ASP
2	B	297	LYS
2	B	298	GLU
2	B	457	ASP
2	B	500	HIS
2	B	564	ARG
2	A	272	ASP
2	A	273	GLU
2	A	361	PRO
2	A	383	ARG
2	B	204	TYR
2	B	361	PRO

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Mol	Chain	Res	Type
2	A	298	GLU
2	A	555	ALA
2	B	272	ASP
2	B	555	ALA
2	A	17	GLY
2	A	281	CYS
2	B	103	LYS
2	B	273	GLU
2	B	518	PRO
2	B	56	GLY
2	B	312	ILE
2	A	56	GLY
2	A	143	VAL
2	B	281	CYS

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	498/503 (99%)	415 (83%)	83 (17%)	2	11
2	B	498/503 (99%)	406 (82%)	92 (18%)	1	7
All	All	996/1006 (99%)	821 (82%)	175 (18%)	2	9

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	8	LEU
2	A	20	ARG
2	A	30	LYS
2	A	42	PRO
2	A	47	VAL
2	A	49	PRO
2	A	59	ILE
2	A	61	ILE
2	A	64	SER

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Mol	Chain	Res	Type
2	A	82	ILE
2	A	85	MET
2	A	89	ASN
2	A	101	LEU
2	A	107	ILE
2	A	108	GLU
2	A	114	ILE
2	A	127	THR
2	A	141	GLN
2	A	143	VAL
2	A	149	THR
2	A	159	ILE
2	A	174	THR
2	A	190	GLU
2	A	198	VAL
2	A	214	ILE
2	A	217	LYS
2	A	222	PRO
2	A	224	ARG
2	A	227	HIS
2	A	229	PHE
2	A	235	ILE
2	A	236	VAL
2	A	243	MET
2	A	264	THR
2	A	268	THR
2	A	277	PHE
2	A	279	CYS
2	A	285	SER
2	A	286	LYS
2	A	287	TYR
2	A	290	GLN
2	A	294	GLU
2	A	295	MET
2	A	297	LYS
2	A	304	LEU
2	A	307	HIS
2	A	316	ILE
2	A	319	VAL
2	A	337	ARG
2	A	340	PRO
2	A	348	ARG

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Mol	Chain	Res	Type
2	A	357	GLU
2	A	359	PHE
2	A	362	ILE
2	A	363	THR
2	A	365	LYS
2	A	368	LEU
2	A	370	LYS
2	A	371	ILE
2	A	372	SER
2	A	380	VAL
2	A	394	ARG
2	A	406	ARG
2	A	407	VAL
2	A	413	LEU
2	A	414	THR
2	A	416	PRO
2	A	429	GLU
2	A	433	LYS
2	A	441	MET
2	A	453	SER
2	A	458	ASP
2	A	460	LYS
2	A	472	VAL
2	A	477	LYS
2	A	499	LEU
2	A	503	LEU
2	A	513	ASN
2	A	529	LYS
2	A	542	ASP
2	A	567	ILE
2	A	568	VAL
2	A	570	GLN
2	B	7	MET
2	B	12	ILE
2	B	20	ARG
2	B	21	ILE
2	B	36	ILE
2	B	44	GLN
2	B	59	ILE
2	B	61	ILE
2	B	80	LEU
2	B	94	VAL

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Mol	Chain	Res	Type
2	B	111	ASN
2	B	114	ILE
2	B	115	ILE
2	B	119	HIS
2	B	127	THR
2	B	131	ILE
2	B	144	LYS
2	B	147	GLU
2	B	159	ILE
2	B	161	GLU
2	B	162	ILE
2	B	163	PRO
2	B	164	MET
2	B	172	THR
2	B	175	ASP
2	B	178	ARG
2	B	185	SER
2	B	190	GLU
2	B	191	ILE
2	B	201	LEU
2	B	217	LYS
2	B	221	ARG
2	B	227	HIS
2	B	229	PHE
2	B	236	VAL
2	B	241	VAL
2	B	252	SER
2	B	260	ASP
2	B	270	ARG
2	B	275	ASP
2	B	282	PRO
2	B	292	LEU
2	B	295	MET
2	B	302	ARG
2	B	306	LEU
2	B	311	VAL
2	B	318	ARG
2	B	324	LYS
2	B	328	LEU
2	B	330	ARG
2	B	332	VAL
2	B	350	LEU

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Mol	Chain	Res	Type
2	B	359	PHE
2	B	361	PRO
2	B	362	ILE
2	B	363	THR
2	B	370	LYS
2	B	371	ILE
2	B	380	VAL
2	B	381	VAL
2	B	389	LYS
2	B	397	GLU
2	B	402	PRO
2	B	403	ILE
2	B	406	ARG
2	B	411	LEU
2	B	412	SER
2	B	413	LEU
2	B	414	THR
2	B	416	PRO
2	B	417	PHE
2	B	419	GLN
2	B	421	GLU
2	B	440	VAL
2	B	446	TYR
2	B	465	LYS
2	B	466	THR
2	B	478	ARG
2	B	479	LEU
2	B	488	LEU
2	B	490	THR
2	B	501	ARG
2	B	507	ARG
2	B	519	PHE
2	B	531	VAL
2	B	532	ILE
2	B	538	ILE
2	B	540	PRO
2	B	542	ASP
2	B	570	GLN
2	B	577	VAL
2	B	582	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	41	ASN
2	A	89	ASN
2	A	118	GLN
2	A	119	HIS
2	A	141	GLN
2	A	165	ASN
2	A	169	GLN
2	A	308	ASN
2	A	321	GLN
2	A	339	HIS
2	A	471	GLN
2	A	475	ASN
2	A	500	HIS
2	A	548	ASN
2	A	558	GLN
2	B	41	ASN
2	B	44	GLN
2	B	63	ASN
2	B	141	GLN
2	B	392	ASN
2	B	471	GLN
2	B	475	ASN
2	B	550	ASN
2	B	558	GLN
2	B	570	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	76/77 (98%)	19 (25%)	9 (11%)
1	D	69/77 (89%)	18 (26%)	6 (8%)
All	All	145/154 (94%)	37 (25%)	15 (10%)

All (37) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	908	U
1	C	909	G
1	C	914	A
1	C	915	G
1	C	916	U
1	C	917	U

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Mol	Chain	Res	Type
1	C	918	G
1	C	924	G
1	C	935	U
1	C	936	A
1	C	938	G
1	C	949	C
1	C	950	C
1	C	960	G
1	C	961	U
1	C	962	C
1	C	963	C
1	C	976	C
1	C	977	A
1	D	908	U
1	D	909	G
1	D	910	G
1	D	914	A
1	D	915	G
1	D	916	U
1	D	917	U
1	D	936	A
1	D	938	G
1	D	946	G
1	D	947	G
1	D	950	C
1	D	960	G
1	D	961	U
1	D	962	C
1	D	963	C
1	D	976	C
1	D	977	A

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	907	G
1	C	913	U
1	C	914	A
1	C	915	G
1	C	916	U
1	C	949	C
1	C	959	A

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Mol	Chain	Res	Type
1	C	961	U
1	C	976	C
1	D	907	G
1	D	913	U
1	D	914	A
1	D	916	U
1	D	959	A
1	D	976	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	77/77 (100%)	-0.58	0	100	100	56, 108, 141, 168	0
1	D	71/77 (92%)	-0.27	0	100	100	76, 150, 198, 200	0
2	A	576/582 (98%)	-0.44	5 (0%)	81	65	32, 74, 121, 162	0
2	B	576/582 (98%)	-0.39	2 (0%)	90	82	27, 70, 115, 142	0
All	All	1300/1318 (98%)	-0.42	7 (0%)	87	76	27, 76, 137, 200	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	62	THR	2.8
2	B	286	LYS	2.6
2	A	102	MET	2.4
2	A	229	PHE	2.3
2	B	296	PRO	2.2
2	A	206	PHE	2.1
2	A	524	LYS	2.1

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
3	MG	B	1601	1/1	0.57	0.14	83,83,83,83	0
3	MG	A	601	1/1	0.91	0.07	85,85,85,85	0
3	MG	B	602	1/1	0.96	0.15	38,38,38,38	0
3	MG	C	1602	1/1	0.98	0.20	52,52,52,52	0
4	ZN	A	600	1/1	1.00	0.03	76,76,76,76	0
4	ZN	B	600	1/1	1.00	0.01	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.