



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:02 AM GMT

PDB ID : 2F8S  
Title : Crystal structure of Aa-Ago with externally-bound siRNA  
Authors : Yuan, Y.R.; Chen, H.Y.; Patel, D.J.  
Deposited on : 2005-12-03  
Resolution : 3.00 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

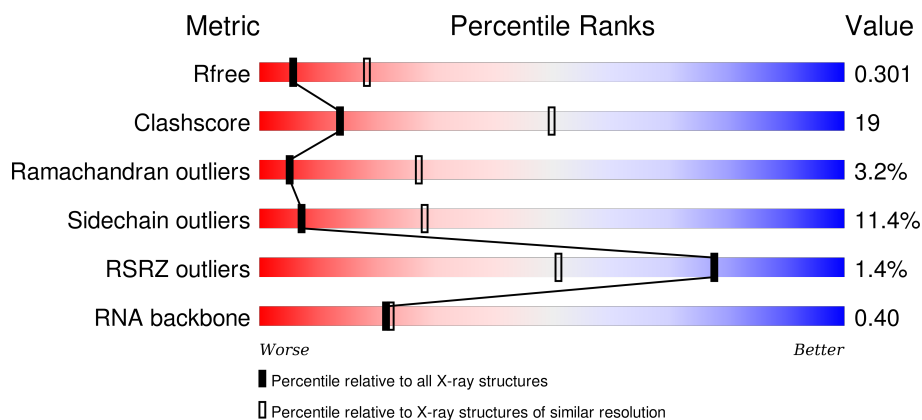
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	22	<div> <div>14%</div> <div>50%</div> <div>36%</div> </div>
1	D	22	<div> <div>5%</div> <div>50%</div> <div>50%</div> </div>
2	A	706	<div> <div>%</div> <div>57%</div> <div>36%</div> <div>6%</div> </div>
2	B	706	<div> <div>2%</div> <div>57%</div> <div>38%</div> <div>5%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12688 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 5'-R(P\*AP\*GP\*AP\*CP\*AP\*GP\*CP\*AP\*UP\*AP\*UP\*AP\*UP\*GP\*CP\*UP\*GP\*UP\*CP\*UP\*UP\*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	22	Total	C	N	O	P	0	0	0
			465	208	78	157	22			
1	D	22	Total	C	N	O	P	0	0	0
			465	208	78	157	22			

- Molecule 2 is a protein called Argonaute protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	704	Total	C	N	O	S	0	0	0
			5864	3818	993	1042	11			
2	B	704	Total	C	N	O	S	0	0	0
			5864	3818	993	1042	11			

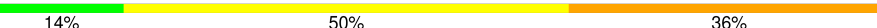
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	17	Total	O	0	0
			17	17		
3	B	13	Total	O	0	0
			13	13		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: 5'-R(P\*AP\*GP\*AP\*CP\*AP\*GP\*CP\*AP\*UP\*AP\*UP\*AP\*UP\*GP\*CP\*UP\*GP\*UP\*CP\*UP\*UP\*U)-3'

Chain C: 



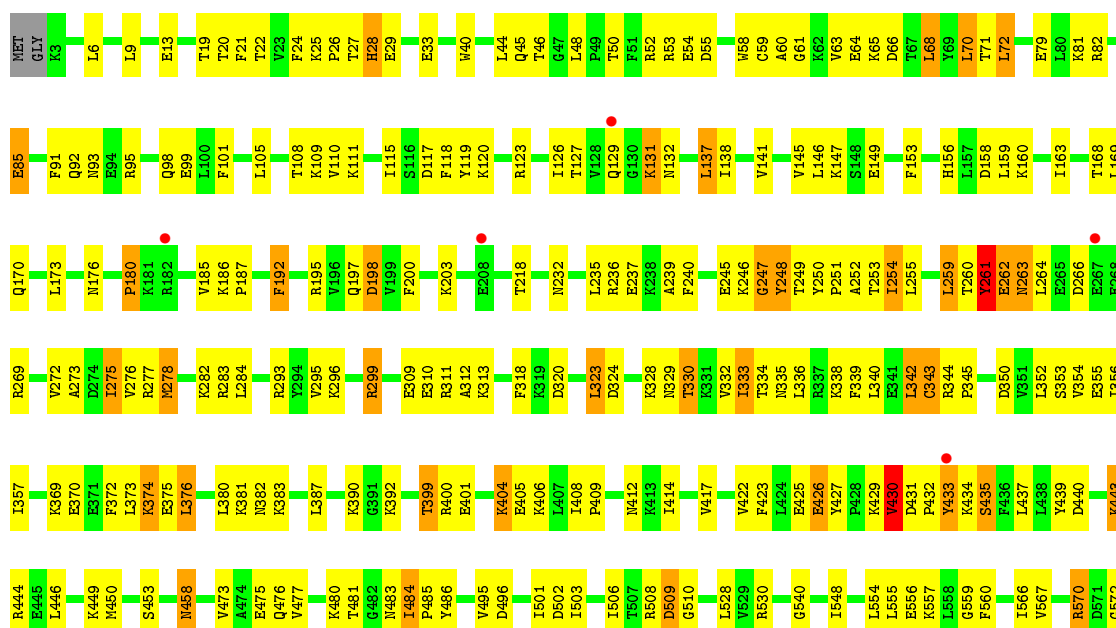
- Molecule 1: 5'-R(P\*AP\*GP\*AP\*CP\*AP\*GP\*CP\*AP\*UP\*AP\*UP\*AP\*UP\*GP\*CP\*UP\*GP\*UP\*CP\*UP\*UP\*U)-3'

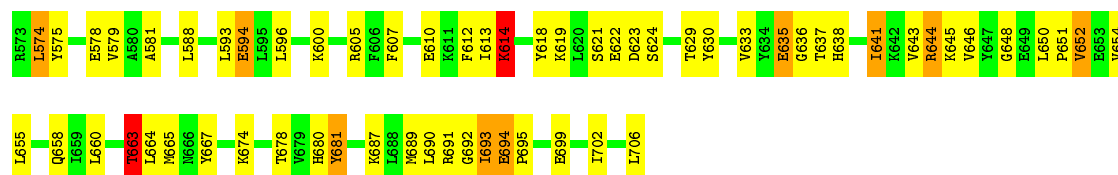
Chain D: 



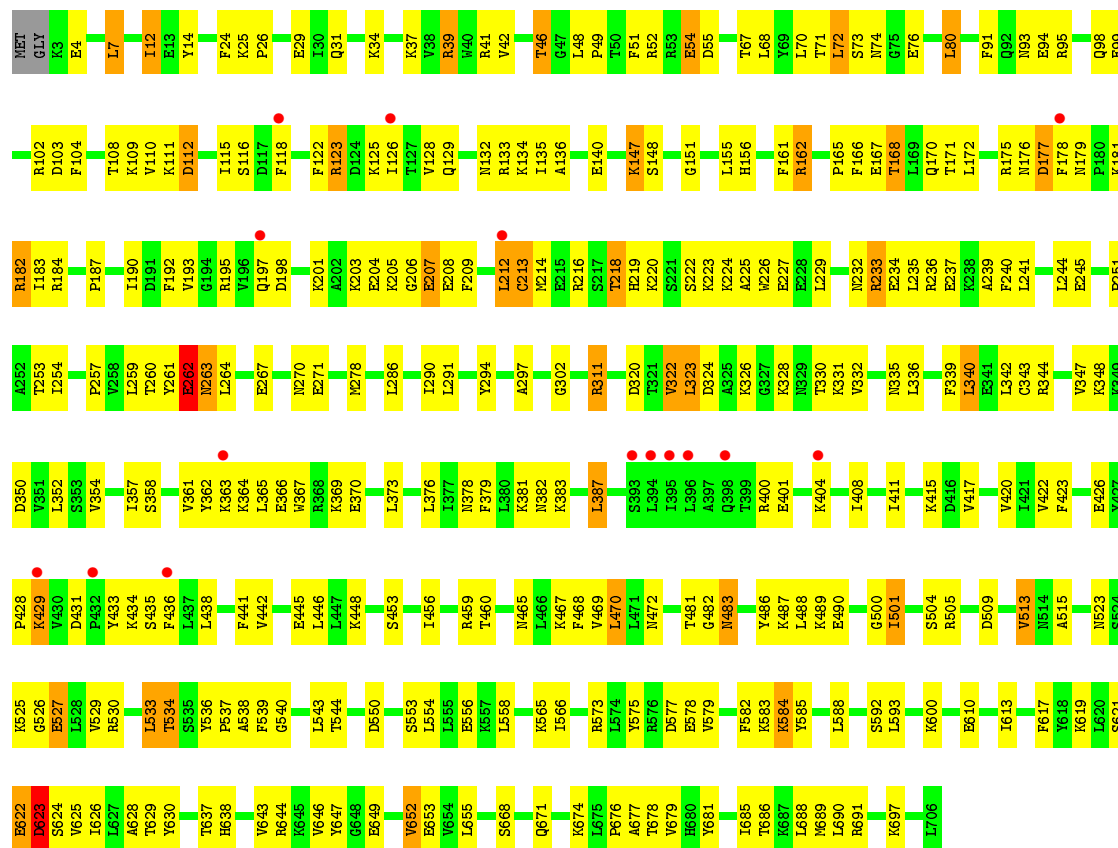
- Molecule 2: Argonaute protein

Chain A: 





• Molecule 2: Argonaute protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.70 Å 117.52 Å 98.62 Å 90.00° 99.12° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 44.06 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.6 (40.00-3.00) 95.6 (44.06-3.00)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.00 (at 3.01 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.212 , 0.307 0.210 , 0.301	Depositor DCC
$R_{free}$ test set	1741 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	69.5	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 77.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 34435 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12688	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.92	16/518 (3.1%)	1.95	19/802 (2.4%)
1	D	2.04	14/518 (2.7%)	1.87	20/802 (2.5%)
2	A	0.74	0/5979	0.82	2/8027 (0.0%)
2	B	0.70	0/5979	0.82	3/8027 (0.0%)
All	All	0.89	30/12994 (0.2%)	0.97	44/17658 (0.2%)

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
2	A	0	1
2	B	0	1
All	All	0	2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	18	U	N1-C6	15.08	1.51	1.38
1	D	18	U	N3-C4	14.51	1.51	1.38
1	C	4	C	N1-C6	14.40	1.45	1.37
1	D	18	U	C2-O2	13.90	1.34	1.22
1	C	6	G	C6-O6	11.80	1.34	1.24
1	C	4	C	N3-C4	11.14	1.41	1.33
1	D	18	U	N1-C2	10.58	1.48	1.38
1	C	6	G	N9-C8	10.38	1.45	1.37
1	D	1	A	OP3-P	-10.13	1.49	1.61
1	C	1	A	OP3-P	-9.96	1.49	1.61
1	C	6	G	N3-C4	9.93	1.42	1.35
1	C	5	A	C5-C6	9.10	1.49	1.41
1	C	4	C	C2-O2	7.77	1.31	1.24
1	D	8	A	N9-C4	7.74	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	6	G	C6-N1	7.60	1.44	1.39
1	C	6	G	C5-C4	7.33	1.43	1.38
1	C	5	A	N9-C4	7.25	1.42	1.37
1	C	5	A	C2-N3	7.14	1.40	1.33
1	D	8	A	N3-C4	6.86	1.39	1.34
1	D	17	G	N7-C5	6.80	1.43	1.39
1	C	6	G	C8-N7	6.69	1.34	1.30
1	D	18	U	C5-C6	6.50	1.40	1.34
1	D	8	A	C6-N1	6.42	1.40	1.35
1	C	5	A	C6-N6	-6.24	1.28	1.33
1	D	11	U	N1-C6	5.31	1.42	1.38
1	D	10	A	N3-C4	5.30	1.38	1.34
1	D	17	G	C6-N1	-5.23	1.35	1.39
1	C	15	C	N1-C6	5.22	1.40	1.37
1	C	4	C	C4-C5	5.15	1.47	1.43
1	D	17	G	N9-C4	5.04	1.42	1.38

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	6	G	C4-C5-N7	13.48	116.19	110.80
1	D	18	U	N3-C4-C5	12.75	122.25	114.60
1	C	6	G	C5-N7-C8	-10.31	99.14	104.30
1	D	18	U	C5-C4-O4	-10.21	119.78	125.90
1	C	6	G	C6-C5-N7	-9.66	124.60	130.40
1	D	18	U	C4-C5-C6	-9.19	114.18	119.70
1	C	6	G	C8-N9-C4	-8.68	102.93	106.40
1	C	6	G	N7-C8-N9	8.23	117.22	113.10
2	A	72	LEU	CA-CB-CG	7.36	132.22	115.30
1	D	18	U	N1-C2-N3	-6.96	110.73	114.90
2	B	623	ASP	CB-CA-C	6.80	124.00	110.40
1	C	4	C	C4-C5-C6	-6.77	114.02	117.40
1	D	3	A	O4'-C1'-N9	6.57	113.46	108.20
1	D	9	U	C4'-C3'-C2'	-6.47	96.13	102.60
1	D	18	U	C6-N1-C2	6.40	124.84	121.00
1	D	11	U	O4'-C1'-N1	6.24	113.19	108.20
1	C	5	A	P-O3'-C3'	6.17	127.10	119.70
1	D	5	A	O4'-C4'-C3'	-6.07	97.93	104.00
1	D	21	U	C4'-C3'-C2'	-6.05	96.55	102.60
1	C	5	A	C2-N3-C4	5.98	113.59	110.60
1	D	7	C	O4'-C1'-N1	5.89	112.91	108.20
1	D	10	A	O4'-C1'-N9	5.87	112.90	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	17	G	N3-C2-N2	-5.84	115.81	119.90
1	D	5	A	C3'-C2'-C1'	-5.77	96.89	101.50
1	C	20	U	C3'-C2'-C1'	-5.47	97.12	101.50
1	C	4	C	N1-C2-O2	5.47	122.18	118.90
1	C	17	G	O4'-C1'-N9	5.42	112.54	108.20
1	D	20	U	P-O3'-C3'	5.41	126.19	119.70
1	D	5	A	P-O3'-C3'	-5.40	113.22	119.70
1	C	6	G	O4'-C1'-N9	5.36	112.48	108.20
1	C	15	C	P-O3'-C3'	-5.29	113.35	119.70
1	C	3	A	C4'-C3'-C2'	-5.25	97.35	102.60
1	D	6	G	O4'-C4'-C3'	-5.25	98.75	104.00
1	D	18	U	N3-C2-O2	5.24	125.87	122.20
2	B	7	LEU	CA-CB-CG	5.17	127.19	115.30
1	C	4	C	N1-C2-N3	-5.13	115.61	119.20
1	C	19	C	N1-C1'-C2'	-5.12	106.36	112.00
1	D	19	C	C6-N1-C2	-5.11	118.26	120.30
1	C	8	A	O4'-C1'-N9	5.10	112.28	108.20
1	D	3	A	P-O3'-C3'	-5.10	113.58	119.70
2	A	588	LEU	CA-CB-CG	5.06	126.93	115.30
1	C	21	U	C3'-C2'-C1'	-5.05	97.46	101.50
1	C	12	A	O4'-C1'-N9	5.04	112.23	108.20
2	B	470	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	176	ASN	Peptide
2	B	623	ASP	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	465	0	233	15	0
1	D	465	0	235	24	0
2	A	5864	0	6128	216	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5864	0	6128	220	0
3	A	17	0	0	0	0
3	B	13	0	0	0	0
All	All	12688	0	12724	468	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 19.

All (468) 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:4:GLU:OE2	2:B:311:ARG:HD3	1.50	1.12
2:B:170:GLN:HE22	2:B:239:ALA:HA	1.13	1.09
2:B:544:THR:HG21	2:B:577:ASP:HB3	1.37	1.07
2:B:575:TYR:HB2	2:B:578:GLU:HG3	1.39	1.05
2:B:170:GLN:NE2	2:B:239:ALA:HA	1.72	1.04
2:A:605:ARG:HH12	2:A:637:THR:CG2	1.76	0.98
2:B:187:PRO:HG2	2:B:190:ILE:HB	1.46	0.98
2:A:693:ILE:O	2:A:694:GLU:HB3	1.65	0.96
2:B:404:LYS:HZ3	2:B:436:PHE:HB2	1.31	0.94
2:A:605:ARG:HH12	2:A:637:THR:HG23	1.32	0.94
2:A:614:LYS:NZ	2:A:663:THR:HG21	1.82	0.94
2:B:46:THR:HG22	2:B:48:LEU:H	1.33	0.94
2:A:131:LYS:HG3	2:A:132:ASN:H	1.34	0.92
1:C:21:U:O4	2:A:123:ARG:NH1	2.03	0.92
2:A:401:GLU:O	2:A:405:GLU:HG3	1.69	0.92
2:B:415:LYS:O	2:B:417:VAL:HG23	1.72	0.90
2:B:232:ASN:HD22	2:B:235:LEU:HG	1.36	0.89
2:B:72:LEU:HD12	2:B:73:SER:H	1.36	0.87
2:B:404:LYS:NZ	2:B:436:PHE:HB2	1.88	0.87
2:B:122:PHE:HE2	2:B:161:PHE:HE2	1.23	0.86
2:B:431:ASP:CB	2:B:434:LYS:HB2	2.04	0.86
2:B:540:GLY:O	2:B:543:LEU:HG	1.76	0.86
2:A:98:GLN:HE21	2:A:145:VAL:H	1.21	0.85
2:B:134:LYS:HB3	2:B:166:PHE:HB2	1.56	0.84
2:A:425:GLU:HG2	2:A:426:GLU:H	1.42	0.84
2:A:295:VAL:O	2:A:299:ARG:HG2	1.78	0.84
2:B:232:ASN:ND2	2:B:235:LEU:HG	1.91	0.84
2:B:431:ASP:HB2	2:B:434:LYS:O	1.77	0.84
1:C:12:A:C2	1:D:10:A:C2	2.65	0.83
2:B:108:THR:HG21	2:B:297:ALA:HB1	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:VAL:O	2:B:46:THR:HB	1.79	0.82
2:B:206:GLY:C	2:B:208:GLU:H	1.83	0.82
2:B:122:PHE:CE2	2:B:161:PHE:HE2	1.97	0.82
2:B:619:LYS:HE2	2:B:653:GLU:OE2	1.79	0.81
2:A:596:LEU:HD11	2:A:655:LEU:HB3	1.63	0.81
2:B:322:VAL:HG13	2:B:486:TYR:HB2	1.60	0.81
2:B:93:ASN:HB3	2:B:95:ARG:H	1.45	0.80
2:A:614:LYS:HG2	2:A:629:THR:O	1.81	0.80
1:D:18:U:H2'	1:D:19:C:H6	1.45	0.79
2:A:614:LYS:HZ2	2:A:663:THR:HG21	1.47	0.79
2:A:400:ARG:HG2	2:A:427:TYR:HB2	1.64	0.79
1:C:20:U:OP2	1:C:22:U:H5'	1.81	0.79
2:B:364:LYS:O	2:B:367:TRP:HB3	1.82	0.78
2:A:339:PHE:O	2:A:343:CYS:HB3	1.84	0.78
2:B:261:TYR:C	2:B:263:ASN:H	1.88	0.77
2:A:335:ASN:HB2	2:A:338:LYS:HB3	1.67	0.77
2:A:369:LYS:HE2	2:A:458:ASN:ND2	2.00	0.76
1:D:12:A:H2'	1:D:13:U:C6	2.21	0.76
2:B:332:VAL:HG22	2:B:336:LEU:HD21	1.68	0.76
2:B:134:LYS:HE3	2:B:167:GLU:HG3	1.68	0.75
2:B:147:LYS:HG2	2:B:621:SER:HB3	1.68	0.75
2:B:357:ILE:O	2:B:422:VAL:HA	1.86	0.75
2:B:52:ARG:HB3	2:B:95:ARG:HH21	1.50	0.75
2:B:446:LEU:HD12	2:B:453:SER:HB2	1.69	0.75
2:A:425:GLU:HG2	2:A:426:GLU:N	2.02	0.74
2:A:232:ASN:HB3	2:A:235:LEU:HG	1.68	0.74
2:A:614:LYS:HZ1	2:A:663:THR:HG21	1.53	0.74
2:B:336:LEU:O	2:B:340:LEU:HB2	1.88	0.74
2:B:685:ILE:O	2:B:689:MET:HB2	1.88	0.74
2:A:40:TRP:CH2	2:A:44:LEU:HD21	2.22	0.73
2:B:232:ASN:HD22	2:B:235:LEU:CG	2.02	0.73
2:A:6:LEU:HD13	2:A:309:GLU:HB2	1.72	0.72
2:A:330:THR:HA	2:A:333:ILE:CG1	2.20	0.72
2:B:536:TYR:OH	2:B:550:ASP:OD2	2.07	0.71
1:D:11:U:H2'	1:D:12:A:C8	2.25	0.71
2:B:431:ASP:HB2	2:B:434:LYS:HB2	1.72	0.71
2:B:108:THR:O	2:B:109:LYS:HB2	1.90	0.71
1:D:16:U:H2'	1:D:17:G:C8	2.26	0.71
2:B:222:SER:O	2:B:226:TRP:HD1	1.73	0.71
2:A:352:LEU:HD21	2:A:481:THR:HG21	1.74	0.70
2:A:24:PHE:HZ	2:A:63:VAL:HG11	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:476:GLN:HB3	2:A:480:LYS:HE3	1.73	0.70
2:A:437:LEU:HD12	2:A:440:ASP:OD2	1.90	0.70
2:A:40:TRP:CZ2	2:A:44:LEU:HD21	2.27	0.70
2:B:431:ASP:HB3	2:B:434:LYS:HB2	1.72	0.70
2:A:330:THR:HA	2:A:333:ILE:HD12	1.74	0.70
2:A:131:LYS:HG3	2:A:132:ASN:N	2.06	0.69
2:A:660:LEU:O	2:A:663:THR:HB	1.93	0.69
2:B:225:ALA:HB2	2:B:254:ILE:HD12	1.75	0.69
2:A:232:ASN:CB	2:A:235:LEU:HG	2.23	0.69
2:B:446:LEU:HD12	2:B:453:SER:CB	2.23	0.68
2:B:646:VAL:O	2:B:647:TYR:HB3	1.92	0.68
2:A:352:LEU:CD2	2:A:481:THR:HG21	2.24	0.68
2:A:108:THR:O	2:A:109:LYS:HB2	1.94	0.68
2:A:356:ILE:HG22	2:A:392:LYS:HG3	1.76	0.67
2:B:24:PHE:CE2	2:B:68:LEU:HG	2.30	0.67
2:A:483:ASN:O	2:A:484:ILE:C	2.33	0.67
2:B:623:ASP:OD1	2:B:623:ASP:N	2.27	0.67
2:B:500:GLY:HA3	2:B:678:THR:HG22	1.77	0.66
2:A:98:GLN:NE2	2:A:145:VAL:H	1.91	0.66
2:A:330:THR:HA	2:A:333:ILE:HB	1.78	0.66
2:A:691:ARG:O	2:A:693:ILE:N	2.29	0.66
2:A:401:GLU:OE2	2:A:430:VAL:HG22	1.96	0.66
2:B:25:LYS:HG2	2:B:26:PRO:HD2	1.76	0.66
2:B:578:GLU:O	2:B:582:PHE:HD1	1.79	0.66
2:A:185:VAL:HG11	2:A:255:LEU:HB3	1.78	0.65
2:B:575:TYR:HB2	2:B:578:GLU:CG	2.21	0.65
2:B:543:LEU:HD12	2:B:544:THR:H	1.62	0.65
2:A:596:LEU:HD22	2:A:643:VAL:HG13	1.79	0.65
2:B:122:PHE:CE2	2:B:161:PHE:CE2	2.84	0.65
2:B:123:ARG:HA	2:B:126:ILE:HD12	1.78	0.64
2:B:195:ARG:HH22	2:B:691:ARG:NH2	1.95	0.64
2:B:621:SER:O	2:B:622:GLU:CB	2.46	0.64
2:B:233:ARG:CG	2:B:233:ARG:HH11	2.11	0.64
2:B:629:THR:HG21	2:B:674:LYS:O	1.98	0.64
2:A:119:TYR:HD2	2:A:123:ARG:HG3	1.62	0.64
2:B:98:GLN:HE21	2:B:102:ARG:CZ	2.09	0.64
2:A:570:ARG:NH1	2:A:574:LEU:HD23	2.13	0.63
2:B:400:ARG:HB3	2:B:404:LYS:HZ2	1.63	0.63
1:D:12:A:H2'	1:D:13:U:H6	1.63	0.63
2:B:617:PHE:HB2	2:B:625:VAL:CG1	2.29	0.63
2:B:472:ASN:ND2	2:B:671:GLN:HE22	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:264:LEU:HB2	2:A:269:ARG:HG3	1.81	0.63
2:A:693:ILE:O	2:A:694:GLU:CB	2.44	0.63
2:A:645:LYS:HB2	2:A:652:VAL:CG1	2.29	0.63
2:A:192:PHE:HE1	2:A:246:LYS:HD2	1.63	0.63
2:A:570:ARG:HH11	2:A:574:LEU:HD23	1.62	0.62
2:B:366:GLU:HB3	2:B:370:GLU:OE1	2.00	0.62
2:A:203:LYS:HG3	2:A:237:GLU:HG2	1.81	0.62
2:B:446:LEU:CD1	2:B:453:SER:HB2	2.29	0.61
2:B:322:VAL:CG1	2:B:486:TYR:HB2	2.30	0.61
2:B:500:GLY:CA	2:B:678:THR:HG22	2.31	0.61
2:A:19:THR:O	2:A:19:THR:HG22	2.00	0.61
2:B:170:GLN:HE22	2:B:239:ALA:CA	2.02	0.61
2:A:330:THR:HA	2:A:333:ILE:CD1	2.31	0.61
2:A:380:LEU:HD12	2:A:387:LEU:HD11	1.82	0.61
2:B:39:ARG:HE	2:B:99:GLU:HG2	1.65	0.61
2:A:173:LEU:HD22	2:A:180:PRO:HG3	1.84	0.60
2:A:650:LEU:HD23	2:A:651:PRO:HD2	1.83	0.60
2:A:111:LYS:HE3	2:A:141:VAL:HB	1.82	0.60
2:B:205:LYS:HD3	2:B:209:PHE:CD2	2.36	0.60
2:B:93:ASN:HB3	2:B:95:ARG:N	2.17	0.59
2:A:425:GLU:CG	2:A:426:GLU:H	2.13	0.59
2:B:206:GLY:C	2:B:208:GLU:N	2.54	0.59
2:B:147:LYS:NZ	2:B:151:GLY:O	2.26	0.59
2:B:652:VAL:HA	2:B:655:LEU:HD12	1.84	0.59
2:A:137:LEU:HD11	2:A:275:ILE:HD12	1.83	0.59
2:B:179:ASN:HB3	2:B:181:LYS:NZ	2.18	0.59
2:A:163:ILE:HD11	2:A:276:VAL:HG21	1.85	0.59
2:B:543:LEU:HD12	2:B:544:THR:N	2.18	0.59
1:D:16:U:H2'	1:D:17:G:H8	1.68	0.58
2:A:356:ILE:HD13	2:A:373:LEU:HD21	1.86	0.58
2:A:605:ARG:NH1	2:A:637:THR:CG2	2.59	0.58
2:A:624:SER:HB3	2:A:644:ARG:HG3	1.86	0.58
1:C:11:U:H2'	1:C:12:A:C8	2.38	0.58
2:A:330:THR:CA	2:A:333:ILE:HD12	2.34	0.58
2:A:645:LYS:HB2	2:A:652:VAL:HG13	1.86	0.58
1:D:1:A:H2'	1:D:2:G:C8	2.39	0.58
2:B:446:LEU:CD1	2:B:453:SER:CB	2.81	0.58
2:B:286:LEU:O	2:B:290:ILE:HD12	2.02	0.58
2:B:366:GLU:HA	2:B:369:LYS:HB2	1.86	0.58
2:A:310:GLU:OE1	2:A:618:TYR:OH	2.14	0.58
2:A:554:LEU:HD23	2:A:557:LYS:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:596:LEU:HD22	2:A:643:VAL:CG1	2.35	0.57
2:A:644:ARG:CZ	2:A:646:VAL:HG22	2.34	0.57
1:D:18:U:H2'	1:D:19:C:C6	2.34	0.57
2:B:347:VAL:HA	2:B:483:ASN:HB3	1.87	0.57
2:B:381:LYS:C	2:B:383:LYS:H	2.07	0.56
2:B:122:PHE:HE2	2:B:161:PHE:CE2	2.14	0.56
2:B:140:GLU:OE2	2:B:162:ARG:HB2	2.05	0.56
2:A:117:ASP:OD2	2:A:293:ARG:NH1	2.29	0.56
2:A:158:ASP:OD1	2:A:159:LEU:N	2.38	0.56
2:B:241:LEU:HD23	2:B:251:PRO:HA	1.87	0.56
2:B:190:ILE:HG22	2:B:192:PHE:H	1.70	0.56
2:B:122:PHE:O	2:B:126:ILE:HG13	2.05	0.56
2:B:373:LEU:HA	2:B:376:LEU:HD12	1.88	0.56
2:B:52:ARG:HB3	2:B:95:ARG:NH2	2.20	0.56
2:A:330:THR:HA	2:A:333:ILE:CB	2.36	0.56
2:B:423:PHE:HA	2:B:456:ILE:O	2.06	0.55
2:B:445:GLU:OE1	2:B:448:LYS:HD2	2.07	0.55
2:B:554:LEU:O	2:B:558:LEU:HG	2.06	0.55
2:B:201:LYS:HE3	2:B:240:PHE:CZ	2.41	0.55
2:B:179:ASN:HB3	2:B:181:LYS:HZ3	1.71	0.55
2:A:369:LYS:HD3	2:A:423:PHE:HB3	1.89	0.55
2:A:333:ILE:HG23	2:A:336:LEU:HD23	1.89	0.55
2:A:645:LYS:CE	2:A:648:GLY:O	2.55	0.55
2:B:74:ASN:OD1	2:B:76:GLU:HB2	2.06	0.55
2:A:95:ARG:HD2	2:A:99:GLU:OE2	2.06	0.55
2:A:369:LYS:HE2	2:A:458:ASN:HD21	1.72	0.55
2:B:328:LYS:HZ2	2:B:342:LEU:HB2	1.71	0.54
2:A:530:ARG:HD2	2:A:699:GLU:OE1	2.07	0.54
2:A:197:GLN:OE1	2:A:245:GLU:HA	2.08	0.54
2:A:338:LYS:O	2:A:342:LEU:HD12	2.07	0.54
2:B:147:LYS:HG2	2:B:621:SER:CB	2.38	0.54
2:B:233:ARG:NH1	2:B:236:ARG:HH12	2.04	0.54
2:A:481:THR:HG22	2:A:481:THR:O	2.08	0.54
2:B:261:TYR:HA	2:B:264:LEU:HD12	1.90	0.54
2:B:233:ARG:HG2	2:B:233:ARG:HH11	1.73	0.54
2:B:438:LEU:O	2:B:442:VAL:HG23	2.08	0.54
2:A:594:GLU:OE1	2:A:650:LEU:HD12	2.08	0.54
2:B:222:SER:O	2:B:226:TRP:CD1	2.58	0.54
1:D:17:G:C2	1:D:18:U:C2	2.96	0.54
2:B:533:LEU:HD21	2:B:689:MET:HG2	1.88	0.54
2:A:13:GLU:OE2	2:B:592:SER:HB2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:352:LEU:CD2	2:B:481:THR:HG21	2.38	0.53
2:A:680:HIS:O	2:A:681:TYR:HB2	2.08	0.53
2:A:170:GLN:NE2	2:A:252:ALA:HB3	2.23	0.53
2:B:332:VAL:HG12	2:B:332:VAL:O	2.09	0.53
2:A:425:GLU:CG	2:A:426:GLU:N	2.70	0.53
2:A:429:LYS:O	2:A:430:VAL:HB	2.08	0.53
2:B:326:LYS:HE3	2:B:344:ARG:HD3	1.91	0.53
2:A:66:ASP:HA	2:A:82:ARG:HD2	1.90	0.53
2:A:248:TYR:HB3	2:A:250:TYR:CE1	2.45	0.53
2:B:619:LYS:CE	2:B:653:GLU:OE2	2.52	0.52
1:D:16:U:H2'	1:D:17:G:O4'	2.09	0.52
2:A:118:PHE:HE2	2:A:126:ILE:HD11	1.74	0.52
2:A:203:LYS:HB2	2:A:237:GLU:HA	1.91	0.52
2:B:203:LYS:O	2:B:204:GLU:HG3	2.09	0.52
2:A:496:ASP:O	2:A:560:PHE:HE2	1.93	0.52
2:A:408:ILE:O	2:A:412:ASN:HB2	2.10	0.52
1:C:19:C:O2'	1:C:20:U:H5'	2.09	0.52
2:A:118:PHE:CE2	2:A:126:ILE:HD11	2.45	0.52
2:A:645:LYS:HE2	2:A:648:GLY:O	2.10	0.52
2:A:613:ILE:O	2:A:614:LYS:C	2.47	0.52
2:B:175:ARG:O	2:B:177:ASP:N	2.43	0.52
2:A:370:GLU:HA	2:A:370:GLU:OE1	2.10	0.52
2:B:4:GLU:CD	2:B:311:ARG:HD3	2.25	0.51
2:B:206:GLY:O	2:B:208:GLU:N	2.39	0.51
2:A:374:LYS:C	2:A:376:LEU:H	2.13	0.51
2:B:261:TYR:C	2:B:263:ASN:N	2.59	0.51
2:B:373:LEU:O	2:B:376:LEU:HB2	2.10	0.51
2:B:529:VAL:O	2:B:530:ARG:HG3	2.10	0.51
2:B:214:MET:O	2:B:223:LYS:HG2	2.10	0.51
2:B:233:ARG:CG	2:B:233:ARG:NH1	2.73	0.51
2:B:51:PHE:CD1	2:B:51:PHE:C	2.84	0.51
2:A:369:LYS:CE	2:A:458:ASN:HD21	2.24	0.51
1:C:21:U:OP1	1:C:21:U:H6	1.93	0.51
2:B:381:LYS:O	2:B:383:LYS:N	2.44	0.51
2:B:431:ASP:HB2	2:B:434:LYS:CB	2.40	0.50
2:A:329:ASN:O	2:A:333:ILE:HG13	2.11	0.50
2:A:449:LYS:O	2:A:450:MET:HB2	2.10	0.50
2:B:49:PRO:HG2	2:B:104:PHE:CZ	2.46	0.50
2:A:335:ASN:CB	2:A:338:LYS:HB3	2.40	0.50
2:A:9:LEU:HD21	2:A:146:LEU:HD12	1.93	0.50
2:A:27:THR:HG22	2:A:81:LYS:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:185:VAL:CG1	2:A:255:LEU:HB3	2.40	0.50
2:B:501:ILE:CD1	2:B:582:PHE:HZ	2.24	0.50
2:B:108:THR:O	2:B:109:LYS:CB	2.57	0.50
2:A:356:ILE:CD1	2:A:373:LEU:HD21	2.41	0.50
2:B:379:PHE:CZ	2:B:383:LYS:HE2	2.46	0.50
2:B:128:VAL:HG21	2:B:267:GLU:O	2.11	0.50
2:B:401:GLU:HG2	2:B:436:PHE:HE1	1.77	0.50
2:A:502:ASP:C	2:A:503:ILE:HG13	2.31	0.50
2:A:91:PHE:HB2	2:A:153:PHE:HE1	1.77	0.50
2:B:232:ASN:ND2	2:B:235:LEU:H	2.09	0.50
2:B:187:PRO:CG	2:B:190:ILE:HB	2.32	0.50
2:A:694:GLU:HG3	2:A:695:PRO:N	2.27	0.50
2:A:296:LYS:HG3	2:A:299:ARG:NH2	2.26	0.50
2:A:269:ARG:O	2:A:273:ALA:HB2	2.12	0.50
2:A:554:LEU:HA	2:A:557:LYS:HD2	1.94	0.49
2:B:404:LYS:HZ3	2:B:436:PHE:CB	2.15	0.49
1:D:3:A:H2'	1:D:4:C:C6	2.47	0.49
2:B:213:CYS:HA	2:B:216:ARG:HB2	1.93	0.49
2:B:12:ILE:HG13	2:B:155:LEU:HB2	1.94	0.49
2:B:136:ALA:HB2	2:B:166:PHE:CE2	2.48	0.49
1:D:11:U:H2'	1:D:12:A:H8	1.77	0.49
2:B:584:LYS:HG3	2:B:585:TYR:CD1	2.47	0.49
2:B:168:THR:HG23	2:B:170:GLN:H	1.77	0.49
1:C:21:U:H5'	2:A:138:ILE:HG21	1.93	0.49
2:A:654:VAL:O	2:A:658:GLN:HG3	2.13	0.49
2:B:187:PRO:HA	2:B:254:ILE:O	2.12	0.48
2:A:185:VAL:HG12	2:A:186:LYS:N	2.27	0.48
2:A:404:LYS:HG2	2:A:405:GLU:N	2.28	0.48
2:B:411:ILE:HG21	2:B:445:GLU:HB3	1.94	0.48
2:B:167:GLU:HG2	2:B:175:ARG:HH12	1.78	0.48
2:A:19:THR:CG2	2:A:19:THR:O	2.60	0.48
2:A:650:LEU:HD22	2:A:654:VAL:HG11	1.94	0.48
2:B:459:ARG:HG2	2:B:460:THR:N	2.28	0.48
1:D:17:G:N1	1:D:18:U:C2	2.81	0.48
2:A:352:LEU:HD21	2:A:481:THR:CG2	2.41	0.48
2:B:125:LYS:O	2:B:271:GLU:HG2	2.12	0.48
2:A:433:TYR:C	2:A:435:SER:H	2.16	0.48
2:A:24:PHE:CZ	2:A:63:VAL:HG11	2.44	0.48
2:A:59:CYS:O	2:A:61:GLY:N	2.45	0.48
2:B:629:THR:CG2	2:B:629:THR:O	2.57	0.48
2:B:39:ARG:HH22	2:B:103:ASP:CG	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:332:VAL:O	2:A:334:THR:N	2.46	0.48
2:B:134:LYS:NZ	2:B:166:PHE:HB3	2.29	0.48
2:B:336:LEU:HB2	2:B:340:LEU:HD12	1.96	0.48
2:B:98:GLN:NE2	2:B:102:ARG:NH2	2.62	0.48
2:A:406:LYS:O	2:A:409:PRO:HD2	2.12	0.48
2:B:109:LYS:O	2:B:112:ASP:HB2	2.14	0.48
1:D:1:A:H2'	1:D:2:G:H8	1.77	0.48
2:B:504:SER:OG	2:B:686:THR:HG22	2.14	0.48
2:A:101:PHE:CE2	2:A:105:LEU:HD11	2.48	0.48
2:B:624:SER:HB3	2:B:644:ARG:HG3	1.94	0.47
1:D:2:G:H2'	1:D:3:A:C8	2.49	0.47
1:D:10:A:C5	1:D:11:U:C4	3.03	0.47
2:A:373:LEU:HA	2:A:376:LEU:HD23	1.96	0.47
2:B:31:GLN:HB2	2:B:34:LYS:HD2	1.96	0.47
2:A:318:PHE:CE1	2:A:320:ASP:HB3	2.49	0.47
2:B:98:GLN:NE2	2:B:102:ARG:CZ	2.78	0.47
2:A:354:VAL:HG21	2:A:387:LEU:HD22	1.97	0.47
2:B:183:ILE:HG22	2:B:184:ARG:N	2.30	0.47
2:B:354:VAL:HG21	2:B:387:LEU:HD11	1.96	0.47
2:A:610:GLU:HG3	2:A:612:PHE:H	1.78	0.47
2:B:260:THR:HG22	2:B:261:TYR:HD2	1.80	0.47
2:B:515:ALA:HB3	2:B:536:TYR:HB2	1.97	0.47
2:B:550:ASP:O	2:B:554:LEU:HG	2.15	0.47
2:A:137:LEU:CD2	2:A:272:VAL:HG13	2.44	0.47
2:A:607:PHE:N	2:A:607:PHE:CD1	2.83	0.47
2:A:284:LEU:HB2	2:A:607:PHE:CD2	2.50	0.47
2:B:446:LEU:CD1	2:B:453:SER:HB3	2.45	0.47
1:D:15:C:H2'	1:D:16:U:C6	2.50	0.47
2:B:352:LEU:HD22	2:B:481:THR:HG21	1.98	0.46
2:B:361:VAL:HG12	2:B:361:VAL:O	2.15	0.46
2:B:128:VAL:HG12	2:B:129:GLN:N	2.29	0.46
2:A:357:ILE:HD11	2:A:414:ILE:HD11	1.97	0.46
1:C:21:U:O5'	1:C:21:U:C2'	2.63	0.46
2:A:45:GLN:HE21	2:A:70:LEU:HD23	1.81	0.46
2:A:555:LEU:HD13	2:A:566:ILE:HD13	1.98	0.46
2:A:149:GLU:CD	2:A:619:LYS:HD3	2.36	0.46
2:B:621:SER:O	2:B:622:GLU:HB3	2.14	0.46
2:B:638:HIS:HD2	2:B:674:LYS:HB3	1.80	0.46
2:A:277:ARG:HH11	2:A:636:GLY:HA2	1.79	0.46
2:A:578:GLU:O	2:A:581:ALA:HB3	2.15	0.46
1:D:2:G:H2'	1:D:3:A:H8	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:570:ARG:NH2	2:A:578:GLU:OE1	2.49	0.46
2:A:623:ASP:HB3	2:A:645:LYS:HB3	1.98	0.46
2:A:192:PHE:CE1	2:A:246:LYS:HD2	2.47	0.46
2:A:689:MET:CE	2:A:689:MET:HA	2.46	0.46
2:A:399:THR:HG21	2:A:401:GLU:OE1	2.16	0.46
2:A:374:LYS:O	2:A:376:LEU:N	2.49	0.46
2:B:37:LYS:O	2:B:41:ARG:HG2	2.16	0.46
2:A:340:LEU:O	2:A:383:LYS:NZ	2.49	0.46
2:B:500:GLY:HA3	2:B:678:THR:O	2.16	0.45
2:A:323:LEU:HA	2:A:328:LYS:O	2.15	0.45
2:A:630:TYR:OH	2:A:638:HIS:HA	2.17	0.45
2:B:260:THR:H	2:B:263:ASN:HD21	1.65	0.45
2:A:475:GLU:OE2	2:A:486:TYR:OH	2.28	0.45
2:B:468:PHE:N	2:B:468:PHE:CD1	2.84	0.45
2:B:70:LEU:HD11	2:B:80:LEU:HD11	1.98	0.45
2:A:283:ARG:NH1	2:A:605:ARG:NH2	2.64	0.45
2:A:651:PRO:O	2:A:654:VAL:N	2.48	0.45
2:B:468:PHE:HD1	2:B:468:PHE:N	2.15	0.45
2:B:579:VAL:HG12	2:B:583:LYS:HD2	1.99	0.45
2:A:52:ARG:HB3	2:A:95:ARG:HH12	1.82	0.45
2:B:320:ASP:OD2	2:B:331:LYS:HG2	2.17	0.45
2:B:49:PRO:HG2	2:B:104:PHE:CE1	2.51	0.45
2:A:404:LYS:CG	2:A:405:GLU:N	2.79	0.44
2:B:73:SER:HB2	2:B:218:THR:O	2.16	0.44
2:B:197:GLN:OE1	2:B:245:GLU:HG3	2.17	0.44
2:A:548:ILE:HD11	2:A:578:GLU:HG2	1.99	0.44
2:A:556:GLU:O	2:A:559:GLY:HA2	2.16	0.44
2:A:28:HIS:ND1	2:A:28:HIS:C	2.71	0.44
2:A:324:ASP:HB2	2:A:344:ARG:O	2.18	0.44
2:B:566:ILE:O	2:B:593:LEU:HA	2.17	0.44
2:B:358:SER:HB2	2:B:369:LYS:NZ	2.33	0.44
2:B:133:ARG:C	2:B:134:LYS:HG2	2.38	0.44
1:C:9:U:H2'	1:C:10:A:C8	2.53	0.44
2:A:27:THR:HG21	2:A:79:GLU:OE1	2.17	0.44
2:B:408:ILE:HD11	2:B:441:PHE:HZ	1.83	0.44
1:C:19:C:C2'	1:C:20:U:H5'	2.48	0.44
2:B:487:LYS:HE2	2:B:527:GLU:HG3	1.98	0.44
2:B:72:LEU:HD12	2:B:73:SER:N	2.17	0.44
2:A:137:LEU:HD21	2:A:272:VAL:HG13	1.99	0.44
2:A:630:TYR:CE2	2:A:674:LYS:HG3	2.53	0.44
2:B:630:TYR:CD2	2:B:630:TYR:N	2.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:570:ARG:HD3	2:A:572:GLY:O	2.17	0.44
2:A:52:ARG:HB3	2:A:95:ARG:NH1	2.33	0.44
2:A:355:GLU:HB2	2:A:417:VAL:HG11	2.00	0.44
2:B:323:LEU:HD21	2:B:489:LYS:HA	2.00	0.44
2:A:373:LEU:HA	2:A:376:LEU:CD2	2.48	0.44
2:B:537:PRO:O	2:B:539:PHE:CD2	2.71	0.44
1:D:3:A:H2'	1:D:4:C:H6	1.82	0.43
2:B:323:LEU:CD2	2:B:489:LYS:HA	2.47	0.43
2:B:262:GLU:HG3	2:B:262:GLU:H	1.62	0.43
2:B:363:LYS:O	2:B:364:LYS:HG3	2.18	0.43
2:A:46:THR:CG2	2:A:48:LEU:HD12	2.47	0.43
2:B:467:LYS:O	2:B:470:LEU:HB2	2.18	0.43
2:B:533:LEU:O	2:B:697:LYS:HA	2.19	0.43
2:A:50:THR:HA	2:A:58:TRP:O	2.18	0.43
2:A:694:GLU:HG3	2:A:695:PRO:HD2	2.01	0.43
2:B:161:PHE:CD1	2:B:161:PHE:N	2.85	0.43
2:B:624:SER:HA	2:B:643:VAL:O	2.18	0.43
2:B:324:ASP:HB2	2:B:344:ARG:O	2.19	0.43
2:B:41:ARG:HD2	2:B:71:THR:O	2.18	0.43
2:B:278:MET:HB3	2:B:278:MET:HE3	1.75	0.43
1:C:10:A:C2	1:D:12:A:C2	3.07	0.43
2:B:523:ASN:ND2	2:B:527:GLU:HB3	2.33	0.43
2:A:439:TYR:O	2:A:443:LYS:HB2	2.18	0.43
2:B:534:THR:HG23	2:B:697:LYS:HG2	1.99	0.43
2:B:128:VAL:HG12	2:B:129:GLN:H	1.84	0.43
2:A:119:TYR:O	2:A:123:ARG:HB2	2.19	0.43
2:B:622:GLU:OE1	2:B:644:ARG:HD2	2.19	0.43
2:A:22:THR:HG21	2:A:63:VAL:HB	1.99	0.43
2:A:665:MET:O	2:A:667:TYR:CD1	2.72	0.43
2:B:224:LYS:HA	2:B:227:GLU:HB3	2.01	0.43
2:A:357:ILE:O	2:A:422:VAL:HA	2.18	0.43
1:C:5:A:N6	1:D:16:U:H3	2.17	0.42
2:A:575:TYR:O	2:A:579:VAL:HG23	2.19	0.42
2:A:508:ARG:O	2:A:510:GLY:N	2.51	0.42
2:B:381:LYS:C	2:B:383:LYS:N	2.71	0.42
2:A:45:GLN:NE2	2:A:70:LEU:HD23	2.33	0.42
2:A:239:ALA:C	2:A:240:PHE:HD1	2.23	0.42
2:B:523:ASN:C	2:B:523:ASN:OD1	2.58	0.42
2:A:437:LEU:HB2	2:A:440:ASP:HB2	2.01	0.42
2:A:261:TYR:OH	2:A:273:ALA:CB	2.68	0.42
2:B:565:LYS:HD2	2:B:592:SER:OG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:635:GLU:H	2:A:635:GLU:HG3	1.63	0.42
2:B:260:THR:HG22	2:B:261:TYR:CD2	2.55	0.42
2:A:574:LEU:HD12	2:A:646:VAL:HG21	2.02	0.42
2:B:348:LYS:HB2	2:B:482:GLY:O	2.19	0.42
2:A:263:ASN:N	2:A:263:ASN:OD1	2.51	0.42
2:A:345:PRO:HB3	2:A:485:PRO:HA	2.01	0.42
2:A:630:TYR:HE2	2:A:674:LYS:HG3	1.85	0.42
2:B:14:TYR:HA	2:B:302:GLY:O	2.20	0.42
2:B:578:GLU:O	2:B:582:PHE:CD1	2.67	0.42
2:A:663:THR:HG22	2:A:664:LEU:HG	2.01	0.42
1:C:21:U:O5'	1:C:21:U:H2'	2.20	0.42
2:A:330:THR:HA	2:A:333:ILE:HG13	2.01	0.42
2:B:534:THR:CG2	2:B:697:LYS:HG2	2.50	0.42
2:A:119:TYR:O	2:A:120:LYS:C	2.57	0.42
1:C:12:A:C2	1:D:10:A:N3	2.87	0.42
2:B:676:PRO:O	2:B:678:THR:N	2.53	0.42
2:B:203:LYS:HE3	2:B:237:GLU:HG2	2.02	0.42
2:A:495:VAL:HG13	2:A:567:VAL:HG23	2.01	0.42
2:A:506:ILE:HD12	2:A:690:LEU:HD22	2.01	0.42
2:B:686:THR:O	2:B:690:LEU:HB2	2.20	0.41
2:B:291:LEU:O	2:B:294:TYR:HB2	2.20	0.41
2:A:694:GLU:HG3	2:A:695:PRO:CD	2.51	0.41
2:A:53:ARG:O	2:A:54:GLU:HB2	2.19	0.41
2:A:372:PHE:O	2:A:373:LEU:C	2.58	0.41
2:A:644:ARG:NH2	2:A:646:VAL:HG22	2.34	0.41
2:A:163:ILE:HG22	2:A:259:LEU:HD12	2.02	0.41
2:B:165:PRO:HG3	2:B:259:LEU:HD11	2.00	0.41
2:A:311:ARG:O	2:A:312:ALA:C	2.56	0.41
2:B:613:ILE:HG22	2:B:628:ALA:HB1	2.02	0.41
2:A:278:MET:SD	2:A:282:LYS:HB3	2.60	0.41
2:A:600:LYS:HA	2:A:641:ILE:HG13	2.02	0.41
2:B:172:LEU:HD11	2:B:257:PRO:HG3	2.02	0.41
2:B:465:ASN:O	2:B:469:VAL:HG23	2.20	0.41
1:C:10:A:C2	1:C:11:U:C2	3.08	0.41
2:A:232:ASN:HB2	2:A:235:LEU:HG	2.00	0.41
2:A:261:TYR:OH	2:A:273:ALA:HB1	2.20	0.41
2:B:115:ILE:O	2:B:115:ILE:HG22	2.20	0.41
2:A:480:LYS:HE2	2:A:706:LEU:C	2.41	0.41
2:B:625:VAL:HG12	2:B:626:ILE:N	2.35	0.41
2:A:261:TYR:O	2:A:269:ARG:HD3	2.21	0.41
2:A:147:LYS:HG3	2:A:153:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:48:LEU:HD13	2:A:61:GLY:HA3	2.03	0.41
2:A:187:PRO:HA	2:A:254:ILE:O	2.20	0.41
2:B:111:LYS:O	2:B:115:ILE:HG13	2.21	0.41
2:A:21:PHE:O	2:A:85:GLU:HA	2.21	0.41
2:B:617:PHE:HB2	2:B:625:VAL:HG13	2.02	0.41
2:A:137:LEU:CD1	2:A:275:ILE:HD12	2.49	0.40
2:B:335:ASN:O	2:B:336:LEU:HD23	2.21	0.40
2:A:261:TYR:HB3	2:A:262:GLU:H	1.73	0.40
2:B:262:GLU:HB2	2:B:435:SER:HB2	2.02	0.40
2:A:313:LYS:HG2	2:A:313:LYS:O	2.21	0.40
2:A:92:GLN:O	2:A:93:ASN:HB3	2.21	0.40
2:A:605:ARG:NH1	2:A:637:THR:HG23	2.16	0.40
2:B:25:LYS:CE	2:B:55:ASP:OD2	2.69	0.40
2:B:629:THR:O	2:B:629:THR:HG22	2.15	0.40
2:A:645:LYS:NZ	2:A:648:GLY:O	2.54	0.40
2:B:358:SER:HB3	2:B:423:PHE:HB2	2.03	0.40
2:A:68:LEU:HA	2:A:68:LEU:HD12	1.92	0.40
2:B:192:PHE:CE1	2:B:219:HIS:CE1	3.10	0.40
2:B:420:VAL:HG12	2:B:422:VAL:HG23	2.03	0.40
2:A:246:LYS:O	2:A:247:GLY:C	2.60	0.40
2:A:353:SER:HB2	2:A:390:LYS:HG3	2.03	0.40
2:A:25:LYS:HA	2:A:26:PRO:HD3	1.92	0.40
1:D:10:A:H2'	1:D:11:U:C6	2.57	0.40
2:B:229:LEU:HD11	2:B:251:PRO:HB3	2.03	0.40
2:A:381:LYS:C	2:A:383:LYS:H	2.24	0.40
2:A:446:LEU:HD13	2:A:453:SER:CB	2.51	0.40
2:A:473:VAL:O	2:A:477:VAL:HG23	2.20	0.40
2:A:431:ASP:HA	2:A:432:PRO:HD3	1.88	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	702/706 (99%)	606 (86%)	73 (10%)	23 (3%)	5	26
2	B	702/706 (99%)	602 (86%)	78 (11%)	22 (3%)	5	28
All	All	1404/1412 (99%)	1208 (86%)	151 (11%)	45 (3%)	5	27

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	60	ALA
2	A	192	PHE
2	A	261	TYR
2	A	430	VAL
2	A	692	GLY
2	A	694	GLU
2	B	176	ASN
2	B	177	ASP
2	B	207	GLU
2	B	343	CYS
2	B	382	ASN
2	B	509	ASP
2	A	131	LYS
2	A	180	PRO
2	A	249	THR
2	A	333	ILE
2	A	434	LYS
2	A	435	SER
2	A	509	ASP
2	A	663	THR
2	A	693	ILE
2	B	54	GLU
2	B	182	ARG
2	B	212	LEU
2	B	244	LEU
2	B	429	LYS
2	B	538	ALA
2	B	677	ALA
2	B	681	TYR
2	A	198	ASP
2	A	247	GLY
2	A	251	PRO
2	A	382	ASN
2	A	614	LYS
2	B	622	GLU

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Mol	Chain	Res	Type
2	A	540	GLY
2	B	270	ASN
2	A	375	GLU
2	A	484	ILE
2	B	262	GLU
2	B	339	PHE
2	B	513	VAL
2	B	679	VAL
2	B	526	GLY
2	B	428	PRO

### 5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	A	646/647 (100%)	573 (89%)	73 (11%)	<b>7</b> 28
2	B	646/647 (100%)	572 (88%)	74 (12%)	<b>7</b> 28
All	All	1292/1294 (100%)	1145 (89%)	147 (11%)	<b>7</b> 28

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	20	THR
2	A	28	HIS
2	A	29	GLU
2	A	33	GLU
2	A	55	ASP
2	A	64	GLU
2	A	65	LYS
2	A	68	LEU
2	A	70	LEU
2	A	71	THR
2	A	72	LEU
2	A	85	GLU
2	A	110	VAL

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Mol	Chain	Res	Type
2	A	115	ILE
2	A	127	THR
2	A	129	GLN
2	A	137	LEU
2	A	156	HIS
2	A	160	LYS
2	A	168	THR
2	A	169	LEU
2	A	195	ARG
2	A	198	ASP
2	A	200	PHE
2	A	218	THR
2	A	236	ARG
2	A	248	TYR
2	A	253	THR
2	A	254	ILE
2	A	259	LEU
2	A	260	THR
2	A	261	TYR
2	A	262	GLU
2	A	263	ASN
2	A	266	ASP
2	A	275	ILE
2	A	278	MET
2	A	299	ARG
2	A	323	LEU
2	A	330	THR
2	A	342	LEU
2	A	343	CYS
2	A	350	ASP
2	A	374	LYS
2	A	376	LEU
2	A	399	THR
2	A	404	LYS
2	A	426	GLU
2	A	430	VAL
2	A	433	TYR
2	A	443	LYS
2	A	444	ARG
2	A	458	ASN
2	A	501	ILE
2	A	509	ASP

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Mol	Chain	Res	Type
2	A	528	LEU
2	A	570	ARG
2	A	574	LEU
2	A	593	LEU
2	A	594	GLU
2	A	614	LYS
2	A	621	SER
2	A	622	GLU
2	A	633	VAL
2	A	635	GLU
2	A	641	ILE
2	A	644	ARG
2	A	652	VAL
2	A	663	THR
2	A	678	THR
2	A	681	TYR
2	A	687	LYS
2	A	702	ILE
2	B	7	LEU
2	B	12	ILE
2	B	29	GLU
2	B	39	ARG
2	B	46	THR
2	B	54	GLU
2	B	67	THR
2	B	72	LEU
2	B	80	LEU
2	B	91	PHE
2	B	94	GLU
2	B	110	VAL
2	B	112	ASP
2	B	116	SER
2	B	118	PHE
2	B	123	ARG
2	B	132	ASN
2	B	135	ILE
2	B	147	LYS
2	B	148	SER
2	B	156	HIS
2	B	162	ARG
2	B	168	THR
2	B	171	THR

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Mol	Chain	Res	Type
2	B	178	PHE
2	B	182	ARG
2	B	193	VAL
2	B	198	ASP
2	B	207	GLU
2	B	212	LEU
2	B	213	CYS
2	B	218	THR
2	B	220	LYS
2	B	233	ARG
2	B	234	GLU
2	B	253	THR
2	B	262	GLU
2	B	263	ASN
2	B	311	ARG
2	B	322	VAL
2	B	323	LEU
2	B	330	THR
2	B	340	LEU
2	B	350	ASP
2	B	362	TYR
2	B	365	LEU
2	B	378	ASN
2	B	387	LEU
2	B	426	GLU
2	B	429	LYS
2	B	433	TYR
2	B	483	ASN
2	B	488	LEU
2	B	490	GLU
2	B	501	ILE
2	B	505	ARG
2	B	513	VAL
2	B	525	LYS
2	B	527	GLU
2	B	533	LEU
2	B	534	THR
2	B	553	SER
2	B	556	GLU
2	B	573	ARG
2	B	584	LYS
2	B	588	LEU

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Mol	Chain	Res	Type
2	B	600	LYS
2	B	610	GLU
2	B	623	ASP
2	B	637	THR
2	B	649	GLU
2	B	652	VAL
2	B	668	SER
2	B	688	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	31	GLN
2	A	98	GLN
2	A	458	ASN
2	A	463	ASN
2	A	569	HIS
2	A	602	ASN
2	A	638	HIS
2	A	658	GLN
2	B	98	GLN
2	B	132	ASN
2	B	164	GLN
2	B	179	ASN
2	B	232	ASN
2	B	263	ASN
2	B	463	ASN
2	B	569	HIS
2	B	632	GLN
2	B	638	HIS
2	B	671	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	21/22 (95%)	6 (28%)	1 (4%)
1	D	21/22 (95%)	6 (28%)	1 (4%)
All	All	42/44 (95%)	12 (28%)	2 (4%)

All (12) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	2	G
1	C	3	A
1	C	11	U
1	C	13	U
1	C	16	U
1	C	22	U
1	D	6	G
1	D	13	U
1	D	14	G
1	D	20	U
1	D	21	U
1	D	22	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	2	G
1	D	21	U

## 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 carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	C	22/22 (100%)	-0.15	0	100	100	66, 79, 103, 107	0
1	D	22/22 (100%)	0.22	1 (4%)	37	15	52, 84, 112, 136	0
2	A	704/706 (99%)	-0.36	5 (0%)	89	70	45, 69, 104, 120	0
2	B	704/706 (99%)	-0.15	15 (2%)	67	36	48, 72, 93, 102	0
All	All	1452/1456 (99%)	-0.25	21 (1%)	78	51	45, 70, 99, 136	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	396	LEU	3.3
1	D	22	U	3.2
2	A	433	TYR	3.2
2	B	395	ILE	3.0
2	A	267	GLU	2.9
2	B	394	LEU	2.9
2	B	398	GLN	2.9
2	B	404	LYS	2.6
2	B	393	SER	2.5
2	B	197	GLN	2.5
2	B	126	ILE	2.5
2	B	212	LEU	2.4
2	B	118	PHE	2.2
2	B	436	PHE	2.2
2	A	208	GLU	2.2
2	B	363	LYS	2.2
2	B	429	LYS	2.2
2	B	178	PHE	2.2
2	B	432	PRO	2.1
2	A	182	ARG	2.1
2	A	129	GLN	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 carbohydrates 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.