



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 26, 2023 – 02:25 PM EDT

PDB ID : 3F73  
Title : Alignment of guide-target seed duplex within an argonaute silencing complex  
Authors : Wang, Y.; Li, H.; Sheng, G.; Juranek, S.; Tuschl, T.; Patel, D.J.  
Deposited on : 2008-11-07  
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

<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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

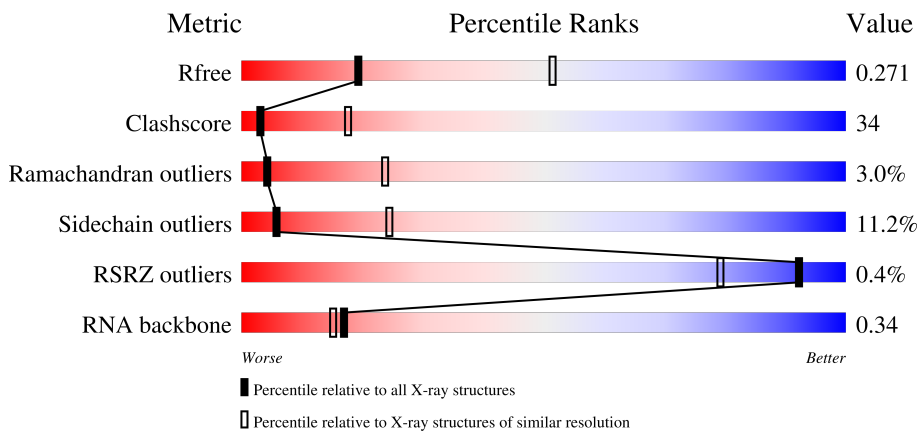
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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.




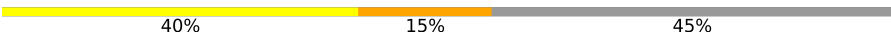
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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  $\geq 3$ , 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	A	685	
1	B	685	
2	C	21	
2	X	21	

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Mol	Chain	Length	Quality of chain
3	H	20	 5% 55% 40%
3	Y	20	 40% 15% 45%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11048 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ARGONAUTE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	678	Total	C	N	O	S	13	0	0
			5075	3261	944	864	6			
1	B	670	Total	C	N	O	S	21	0	0
			4969	3193	912	857	7			

- Molecule 2 is a DNA chain called DNA (5'-D(P\*DTP\*DGP\*DAP\*DGP\*DGP\*DTP\*DAP\*DGP\*DTP\*DAP\*DGP\*DGP\*DTP\*DTP\*DGP\*DTP\*DA\*DTP\*DAP\*DGP\*DT)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	16	Total	C	N	O	P	0	0	1
			292	135	54	88	15			
2	X	15	Total	C	N	O	P	0	0	1
			296	140	55	87	14			

- Molecule 3 is a RNA chain called RNA (5'-R(\*UP\*AP\*UP\*AP\*CP\*AP\*A\*CP\*UP\*CP\*A\*P\*CP\*UP\*AP\*CP\*CP\*UP\*CP\*GP\*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	H	12	Total	C	N	O	P	0	0	1
			203	89	28	75	11			
3	Y	11	Total	C	N	O	P	0	0	1
			189	84	26	69	10			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	X	1	Total	Mg	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	O	0	0
			5	4 1		

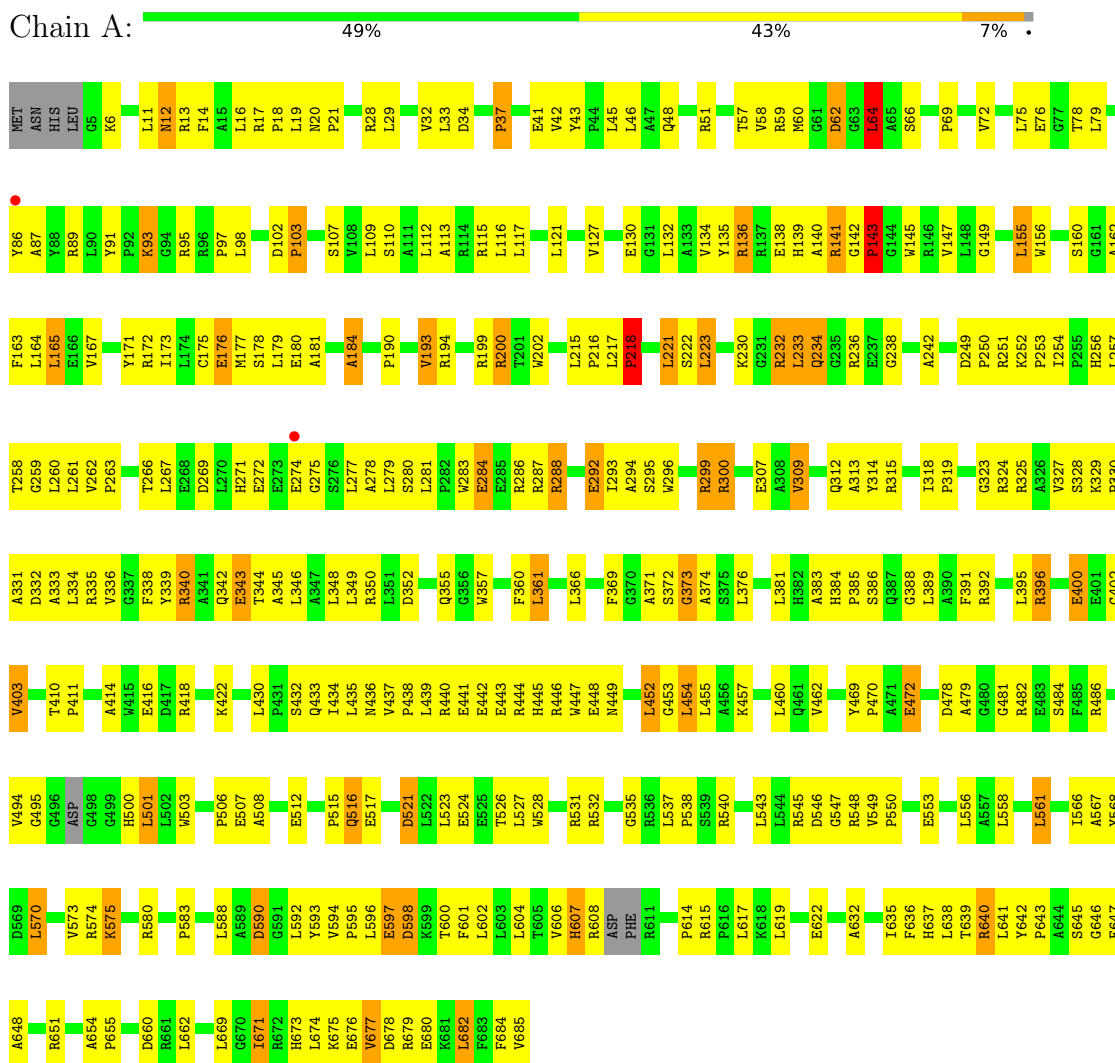
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total	O	0	0
			8	8		
6	B	8	Total	O	0	0
			8	8		

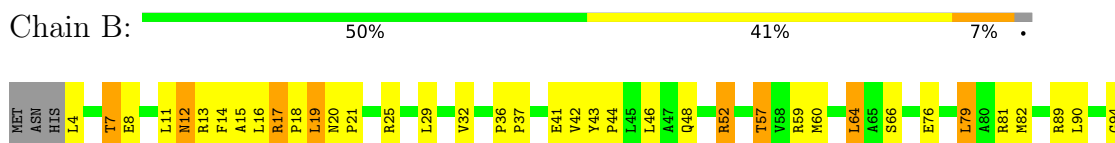
### 3 Residue-property plots

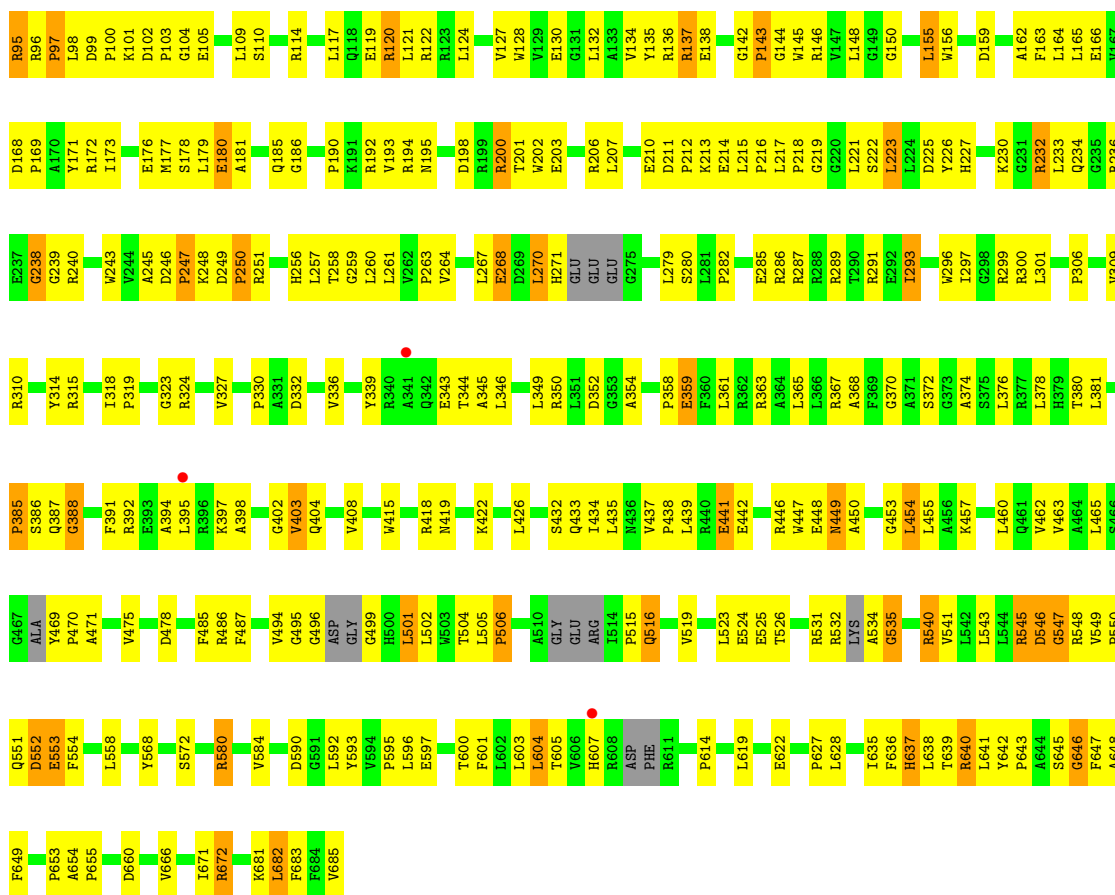
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ARGONAUTE



#### • Molecule 1: ARGONAUTE





- Molecule 2: DNA (5'-D(P\*DTP\*DGP\*DAP\*DGP\*DGP\*DTP\*DAP\*DGP\*DTP\*DAP\*DGP\*DGP\*DTP\*DTP\*DGP\*DTP\*DA\*DTP\*DAP\*DGP\*DT)-3')

Chain C: 5% 43% 24% 5% 24%



- Molecule 2: DNA (5'-D(P\*DTP\*DGP\*DAP\*DGP\*DGP\*DTP\*DAP\*DGP\*DTP\*DAP\*DGP\*DGP\*DTP\*DTP\*DGP\*DTP\*DA\*DTP\*DAP\*DGP\*DT)-3')

Chain X: 38% 19% 14% 29%



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

Chain H: 5% 55% 40%



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

Chain Y:  40% 15% 45%

U A U A C A A C D9 C10 A11 C12 U13 A14 C15 C16 U17 C18 C19 U



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.16Å 120.53Å 109.08Å 90.00° 105.30° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 42.16 – 2.81	Depositor EDS
% Data completeness (in resolution range)	97.3 (30.00-3.00) 95.9 (42.16-2.81)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.09 (at 2.81Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.221 , 0.282 0.215 , 0.271	Depositor DCC
$R_{free}$ test set	2512 reflections (7.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.7	Xtrriage
Anisotropy	0.309	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 54.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11048	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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, 0.333 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: PO4, MG

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	A	0.47	1/5197 (0.0%)	0.78	9/7084 (0.1%)
1	B	0.43	0/5084	0.76	6/6934 (0.1%)
2	C	1.24	2/326 (0.6%)	1.63	7/501 (1.4%)
2	X	1.17	3/331 (0.9%)	1.63	9/508 (1.8%)
3	H	1.02	1/223 (0.4%)	1.15	0/345
3	Y	1.30	3/208 (1.4%)	1.12	2/321 (0.6%)
All	All	0.56	10/11369 (0.1%)	0.87	33/15693 (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	C	0	2
2	X	0	4
All	All	0	6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	18	DT	O3'-P	-12.66	1.46	1.61
3	Y	9	U	O3'-P	-10.62	1.48	1.61
3	Y	10	C	P-OP2	7.39	1.61	1.49
2	X	1	DT	OP3-P	-7.39	1.52	1.61
3	Y	10	C	P-OP1	7.32	1.61	1.49
2	C	1	DT	OP3-P	-7.25	1.52	1.61
3	H	8	C	O3'-P	-6.83	1.52	1.61
2	X	17	DA	O3'-P	-6.82	1.52	1.61
2	X	6	DT	C4-C5	-5.86	1.39	1.45
1	A	221	LEU	C-O	5.31	1.33	1.23

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	10	DA	N9-C1'-C2'	9.36	130.39	112.60
2	C	10	DA	C4-N9-C1'	8.79	142.12	126.30
2	X	9	DT	O3'-P-O5'	8.71	120.56	104.00
2	C	10	DA	C8-N9-C1'	-8.52	112.36	127.70
3	Y	12	C	P-O3'-C3'	-8.52	109.48	119.70
1	A	481	GLY	N-CA-C	-8.02	93.05	113.10
2	X	6	DT	N1-C1'-C2'	7.59	127.03	112.60
2	C	6	DT	N1-C1'-C2'	7.50	126.84	112.60
1	A	598	ASP	N-CA-C	7.42	131.02	111.00
1	A	607	HIS	N-CA-C	-7.16	91.66	111.00
1	B	607	HIS	N-CA-C	-6.74	92.79	111.00
3	Y	10	C	OP1-P-OP2	-6.73	109.51	119.60
2	X	9	DT	N1-C1'-C2'	6.71	125.34	112.60
2	C	9	DT	N1-C1'-C2'	6.62	125.17	112.60
1	B	97	PRO	N-CA-CB	6.05	110.56	103.30
1	A	323	GLY	N-CA-C	-6.02	98.05	113.10
2	X	9	DT	P-O3'-C3'	-5.96	112.55	119.70
1	A	64	LEU	CA-CB-CG	5.77	128.58	115.30
2	C	10	DA	OP1-P-O3'	5.48	117.27	105.20
1	A	506	PRO	N-CA-CB	5.46	109.86	103.30
1	A	97	PRO	N-CA-CB	5.45	109.84	103.30
1	B	385	PRO	N-CA-CB	5.45	109.84	103.30
1	A	355	GLN	N-CA-C	5.41	125.60	111.00
1	B	535	GLY	N-CA-C	5.38	126.55	113.10
2	C	7	DA	O4'-C1'-N9	5.37	111.76	108.00
1	B	506	PRO	N-CA-CB	5.25	109.60	103.30
1	A	561	LEU	CA-CB-CG	5.25	127.36	115.30
1	B	155	LEU	CA-CB-CG	5.16	127.16	115.30
2	X	6	DT	O4'-C1'-C2'	5.15	110.02	105.90
2	X	19	DA	C2'-C3'-O3'	-5.06	95.89	112.60
2	X	1	DT	OP1-P-OP2	-5.06	112.01	119.60
2	X	8	DG	N9-C1'-C2'	5.06	122.21	112.60
2	X	7	DA	O4'-C1'-N9	5.05	111.53	108.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	2	DG	Sidechain
2	C	9	DT	Sidechain
2	X	20	DG	Sidechain

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Mol	Chain	Res	Type	Group
2	X	6	DT	Sidechain
2	X	8	DG	Sidechain
2	X	9	DT	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5075	0	5007	328	2
1	B	4969	0	4842	320	2
2	C	292	0	155	35	0
2	X	296	0	161	40	0
3	H	203	0	107	29	0
3	Y	189	0	99	15	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	X	1	0	0	0	0
5	C	5	0	0	0	0
6	A	8	0	0	1	0
6	B	8	0	0	0	0
All	All	11048	0	10371	718	2

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 34.

All (718) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ASP:OD1	1:B:103:PRO:HD2	1.39	1.19
1:A:561:LEU:HD22	1:A:566:ILE:HD11	1.29	1.15
1:B:545:ARG:HE	1:B:547:GLY:HA2	1.08	1.12
1:A:396:ARG:HH11	1:A:396:ARG:HB3	1.07	1.11
2:C:10:DA:H4'	2:C:11:DG:OP1	1.32	1.09
1:B:136:ARG:HH22	1:B:293:ILE:CG2	1.65	1.07
2:C:8:DG:H2''	2:C:9:DT:H5'	1.38	1.06
2:X:20:DG:H2''	2:X:21:DT:H5'	1.11	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:LEU:HB2	1:B:381:LEU:HD12	1.38	1.06
1:B:494:VAL:HG22	1:B:501:LEU:HB3	1.38	1.05
1:B:136:ARG:HH22	1:B:293:ILE:HG23	1.23	1.03
1:B:114:ARG:HD3	1:B:132:LEU:HD11	1.40	1.02
1:A:575:LYS:H	1:A:575:LYS:HZ2	1.08	1.01
1:B:415:TRP:HE3	1:B:419:ASN:HD21	1.10	0.99
2:X:8:DG:C2'	2:X:9:DT:H5''	1.93	0.98
1:B:501:LEU:HD13	1:B:682:LEU:HD11	1.45	0.97
1:B:280:SER:HA	2:X:7:DA:H5'	1.47	0.96
1:B:287:ARG:HE	1:B:291:ARG:HH12	1.05	0.95
1:B:18:PRO:HA	1:B:162:ALA:HA	1.46	0.94
1:B:545:ARG:HG2	1:B:547:GLY:H	1.33	0.92
1:A:604:LEU:HD11	1:A:614:PRO:HB2	1.49	0.92
1:B:102:ASP:OD1	1:B:103:PRO:CD	2.18	0.91
1:B:12:ASN:HD22	1:B:12:ASN:H	1.15	0.91
1:B:8:GLU:HG3	1:B:584:VAL:HG21	1.53	0.90
2:X:8:DG:H2''	2:X:9:DT:H5''	1.49	0.90
1:A:18:PRO:HA	1:A:162:ALA:HA	1.53	0.90
3:H:16:C:H2'	3:H:17:U:O4'	1.70	0.90
1:A:327:VAL:CG2	1:A:332:ASP:HB2	2.02	0.89
1:A:396:ARG:HB3	1:A:396:ARG:NH1	1.87	0.88
1:B:173:ILE:HG22	2:X:9:DT:OP1	1.72	0.88
1:A:76:GLU:HG2	1:A:89:ARG:HG2	1.55	0.88
1:B:267:LEU:HD12	1:B:267:LEU:O	1.73	0.88
1:A:639:THR:HG22	1:A:640:ARG:HE	1.38	0.87
1:A:469:TYR:HB3	1:A:470:PRO:HD2	1.56	0.87
1:A:494:VAL:HG11	1:A:641:LEU:HD13	1.57	0.87
1:B:287:ARG:HE	1:B:291:ARG:NH1	1.71	0.86
1:B:486:ARG:HG2	1:B:515:PRO:HD3	1.57	0.86
1:B:76:GLU:HG2	1:B:89:ARG:HG2	1.58	0.85
1:B:137:ARG:HH21	1:B:137:ARG:HG3	1.41	0.85
1:A:51:ARG:NH2	1:A:115:ARG:HD3	1.92	0.85
1:B:12:ASN:H	1:B:12:ASN:ND2	1.72	0.85
1:B:289:ARG:O	1:B:293:ILE:HD13	1.76	0.85
1:A:327:VAL:HG21	1:A:332:ASP:HB2	1.56	0.84
1:B:264:VAL:HG11	2:X:10:DA:OP1	1.78	0.84
1:B:437:VAL:HG12	1:B:438:PRO:HD3	1.60	0.83
2:X:20:DG:C2'	2:X:21:DT:H5'	2.04	0.83
1:A:445:HIS:NE2	3:H:18:C:H2'	1.93	0.83
1:B:12:ASN:HD22	1:B:12:ASN:N	1.70	0.83
2:X:20:DG:H2''	2:X:21:DT:C5'	2.05	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:LEU:HD22	1:A:566:ILE:CD1	2.08	0.83
2:C:20:DG:H2''	2:C:21:DT:H5'	1.59	0.83
2:C:10:DA:H2''	2:C:11:DG:H5''	1.59	0.82
3:Y:13:U:H2'	3:Y:14:A:H8	1.43	0.82
1:A:12:ASN:H	1:A:12:ASN:HD22	1.27	0.82
1:A:346:LEU:HD22	1:A:454:LEU:HD13	1.62	0.82
1:A:546:ASP:OD2	1:A:575:LYS:HE2	1.80	0.82
2:C:20:DG:H2''	2:C:21:DT:C5'	2.08	0.81
1:A:20:ASN:HB2	1:A:21:PRO:HD2	1.62	0.81
1:B:280:SER:HA	2:X:7:DA:C5'	2.11	0.81
2:C:8:DG:C2'	2:C:9:DT:H5'	2.11	0.80
2:C:10:DA:C4'	2:C:11:DG:OP1	2.25	0.80
1:A:516:GLN:HB2	1:A:556:LEU:HD23	1.62	0.80
3:Y:13:U:H2'	3:Y:14:A:C8	2.16	0.80
1:B:136:ARG:NH2	1:B:293:ILE:HG23	1.97	0.79
1:A:28:ARG:HD3	1:A:93:LYS:HE3	1.65	0.79
1:B:437:VAL:CG1	1:B:438:PRO:HD3	2.13	0.79
1:B:17:ARG:HG2	1:B:18:PRO:N	1.96	0.79
2:X:2:DG:H2''	2:X:3:DA:C5'	2.13	0.79
1:A:350:ARG:HG2	1:A:352:ASP:OD1	1.83	0.78
1:A:299:ARG:HG2	1:A:299:ARG:HH11	1.48	0.78
1:B:604:LEU:HD21	1:B:614:PRO:HB2	1.65	0.78
1:A:640:ARG:HD2	1:A:640:ARG:N	1.98	0.78
1:A:636:PHE:O	1:A:639:THR:HB	1.83	0.78
1:A:12:ASN:HD22	1:A:12:ASN:N	1.80	0.78
1:A:280:SER:HA	2:C:7:DA:C5'	2.15	0.77
1:A:575:LYS:H	1:A:575:LYS:NZ	1.81	0.77
1:B:190:PRO:HG2	1:B:263:PRO:HB3	1.68	0.77
1:A:75:LEU:O	1:A:76:GLU:HG3	1.85	0.76
1:A:411:PRO:HG3	1:A:437:VAL:HG11	1.67	0.76
3:Y:18:C:H5'	3:Y:19:G:OP1	1.84	0.76
1:B:79:LEU:HD23	1:B:79:LEU:N	2.01	0.76
1:A:325:ARG:HH11	1:A:325:ARG:HB3	1.50	0.75
1:B:173:ILE:N	2:X:9:DT:OP1	2.19	0.75
1:B:545:ARG:NE	1:B:547:GLY:HA2	1.94	0.75
1:A:138:GLU:HB3	1:A:141:ARG:NH2	2.00	0.75
2:X:2:DG:H2''	2:X:3:DA:H5'	1.69	0.75
1:B:415:TRP:HE3	1:B:419:ASN:ND2	1.81	0.75
3:H:11:A:C2'	3:H:12:C:H5'	2.16	0.75
1:A:127:VAL:HG11	1:A:134:VAL:HG13	1.68	0.74
1:B:136:ARG:NH1	1:B:293:ILE:HG13	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:SER:CB	2:C:7:DA:H5'	2.17	0.74
1:A:376:LEU:H	1:A:376:LEU:HD23	1.52	0.73
1:B:103:PRO:HD2	1:B:104:GLY:H	1.52	0.73
1:B:127:VAL:HG11	1:B:134:VAL:HG13	1.69	0.73
1:A:561:LEU:CD2	1:A:566:ILE:HD11	2.15	0.73
1:B:180:GLU:HG2	1:B:258:THR:OG1	1.89	0.73
1:A:180:GLU:HG2	1:A:258:THR:OG1	1.89	0.73
1:A:457:LYS:HE2	1:A:685:VAL:HG23	1.69	0.73
1:A:484:SER:HB2	1:A:553:GLU:OE1	1.89	0.72
1:A:342:GLN:HG3	1:A:343:GLU:H	1.55	0.72
1:B:540:ARG:HH11	1:B:540:ARG:HB2	1.54	0.71
1:B:545:ARG:HE	1:B:547:GLY:CA	1.97	0.71
1:B:279:LEU:O	2:X:7:DA:H4'	1.89	0.71
1:B:136:ARG:HH22	1:B:293:ILE:HG21	1.55	0.71
1:B:415:TRP:HA	1:B:418:ARG:HB3	1.72	0.71
1:B:138:GLU:HA	1:B:148:LEU:HD23	1.72	0.71
1:A:445:HIS:NE2	3:H:18:C:C2'	2.53	0.71
1:B:330:PRO:HB2	1:B:646:GLY:HA2	1.73	0.71
1:B:7:THR:HG22	1:B:8:GLU:H	1.55	0.71
1:A:32:VAL:CG2	1:A:89:ARG:HB2	2.21	0.70
1:A:325:ARG:HB3	1:A:325:ARG:NH1	2.05	0.70
1:B:20:ASN:HB2	1:B:21:PRO:HD2	1.71	0.70
1:A:233:LEU:HD23	1:A:260:LEU:HD21	1.71	0.70
1:A:252:LYS:HD2	1:A:254:ILE:HD11	1.73	0.70
1:A:46:LEU:HD12	1:A:59:ARG:HD2	1.74	0.70
1:A:540:ARG:HA	1:A:567:ALA:O	1.92	0.70
1:B:136:ARG:CZ	1:B:293:ILE:HG13	2.20	0.70
1:B:282:PRO:HG2	1:B:285:GLU:HB2	1.74	0.70
2:X:4:DG:H2'	2:X:5:DG:C8	2.25	0.70
1:A:574:ARG:HA	1:A:575:LYS:HZ1	1.57	0.70
1:A:200:ARG:HD2	1:A:202:TRP:CZ2	2.27	0.69
1:B:494:VAL:HG12	1:B:495:GLY:H	1.56	0.69
1:B:327:VAL:CG2	1:B:332:ASP:HB2	2.21	0.69
3:H:11:A:H2'	3:H:12:C:H5'	1.72	0.69
1:A:156:TRP:HE1	1:A:164:LEU:HD12	1.56	0.69
1:B:496:GLY:C	1:B:499:GLY:HA3	2.13	0.69
1:B:120:ARG:HG3	1:B:301:LEU:HD23	1.75	0.69
1:B:415:TRP:CE3	1:B:419:ASN:ND2	2.61	0.69
1:A:135:TYR:CE2	1:A:172:ARG:HB2	2.28	0.68
1:B:42:VAL:HG13	1:B:43:TYR:HD1	1.58	0.68
1:B:280:SER:CA	2:X:7:DA:H5'	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:VAL:HG13	1:A:43:TYR:HD1	1.58	0.68
1:B:15:ALA:HA	1:B:164:LEU:HD23	1.75	0.68
1:B:190:PRO:HG2	1:B:263:PRO:CB	2.23	0.68
1:A:280:SER:HA	2:C:7:DA:H5''	1.76	0.67
1:A:558:LEU:HD22	1:A:568:TYR:CE2	2.29	0.67
1:A:645:SER:HB2	1:A:648:ALA:O	1.95	0.67
1:A:334:LEU:HD11	1:A:452:LEU:HD13	1.77	0.67
1:A:575:LYS:HD2	3:H:9:U:H5'	1.75	0.67
1:B:645:SER:HB2	1:B:648:ALA:O	1.94	0.67
1:A:639:THR:CG2	1:A:640:ARG:HE	2.08	0.67
2:C:8:DG:H2''	2:C:9:DT:C5'	2.21	0.67
1:B:545:ARG:CG	1:B:547:GLY:H	2.07	0.67
1:B:127:VAL:CG1	1:B:134:VAL:HG13	2.24	0.66
1:B:478:ASP:OD1	1:B:660:ASP:HA	1.96	0.66
2:X:4:DG:H2'	2:X:5:DG:H8	1.59	0.66
2:X:8:DG:H2'	2:X:9:DT:H5''	1.76	0.66
1:A:156:TRP:NE1	1:A:164:LEU:HD12	2.10	0.66
1:B:42:VAL:HG13	1:B:43:TYR:H	1.60	0.66
1:B:572:SER:HB3	1:B:622:GLU:OE2	1.95	0.66
1:B:287:ARG:NE	1:B:291:ARG:HH12	1.84	0.66
3:Y:16:C:O2'	3:Y:17:U:H5'	1.95	0.66
3:H:14:A:H2'	3:H:15:C:H6	1.61	0.66
1:A:330:PRO:HB2	1:A:646:GLY:HA2	1.78	0.65
1:A:283:TRP:HZ3	1:A:287:ARG:HH11	1.44	0.65
1:A:327:VAL:HG22	1:A:328:SER:N	2.11	0.65
1:B:558:LEU:HD22	1:B:568:TYR:CE2	2.31	0.65
1:B:640:ARG:HD2	1:B:640:ARG:N	2.11	0.65
1:B:17:ARG:HG2	1:B:18:PRO:CD	2.27	0.65
1:A:410:THR:O	1:A:436:ASN:HA	1.97	0.65
1:B:172:ARG:HG3	1:B:172:ARG:HH11	1.61	0.65
1:B:494:VAL:HG12	1:B:495:GLY:N	2.11	0.65
1:B:597:GLU:CD	1:B:597:GLU:H	2.00	0.65
3:H:14:A:O2'	3:H:15:C:H5'	1.96	0.64
1:A:437:VAL:O	1:A:439:LEU:N	2.30	0.64
1:A:607:HIS:O	1:A:608:ARG:C	2.35	0.64
1:A:453:GLY:O	1:A:457:LYS:HG3	1.98	0.64
1:B:192:ARG:NH1	2:X:10:DA:H4'	2.13	0.64
1:A:42:VAL:HG13	1:A:43:TYR:H	1.62	0.64
2:X:2:DG:H2''	2:X:3:DA:O5'	1.98	0.64
1:A:19:LEU:HD22	1:A:109:LEU:HD13	1.80	0.63
1:B:267:LEU:HD22	3:Y:13:U:O4'	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:GLN:CG	1:A:343:GLU:N	2.61	0.63
1:A:138:GLU:HB3	1:A:141:ARG:HH22	1.60	0.63
1:A:78:THR:HA	1:A:86:TYR:O	1.99	0.63
1:A:339:TYR:CE2	1:A:340:ARG:HD3	2.33	0.63
1:B:57:THR:HB	1:B:66:SER:HB2	1.80	0.63
1:B:672:ARG:HG3	1:B:672:ARG:HH11	1.64	0.63
1:A:345:ALA:O	1:A:403:VAL:HA	1.98	0.63
3:H:11:A:H2'	3:H:12:C:C5'	2.28	0.63
1:B:137:ARG:HG3	1:B:137:ARG:NH2	2.08	0.62
1:B:177:MET:HG3	1:B:181:ALA:HB3	1.79	0.62
1:B:435:LEU:HD13	1:B:450:ALA:HB2	1.81	0.62
1:B:465:LEU:HD13	1:B:469:TYR:OH	1.99	0.62
3:H:11:A:O2'	3:H:12:C:H5'	1.98	0.62
1:A:396:ARG:HH11	1:A:396:ARG:CB	1.98	0.62
1:B:173:ILE:HG23	1:B:173:ILE:O	1.99	0.62
1:B:640:ARG:HG3	1:B:649:PHE:CE2	2.35	0.62
3:H:16:C:C2'	3:H:17:U:H5'	2.29	0.62
1:A:12:ASN:H	1:A:12:ASN:ND2	1.96	0.62
1:A:217:LEU:O	1:A:218:PRO:C	2.37	0.62
1:B:48:GLN:HG3	2:X:18:DT:H1'	1.81	0.62
1:B:471:ALA:HA	1:B:540:ARG:HB3	1.80	0.62
1:B:238:GLY:HA2	1:B:259:GLY:HA3	1.81	0.62
1:A:215:LEU:HD22	1:A:216:PRO:HD2	1.82	0.61
1:A:256:HIS:HD2	1:A:257:LEU:H	1.49	0.61
1:B:203:GLU:HG2	1:B:247:PRO:HG3	1.82	0.61
1:B:185:GLN:O	1:B:185:GLN:HG3	2.00	0.61
1:B:475:VAL:CG1	1:B:543:LEU:HD23	2.31	0.61
1:B:46:LEU:HB3	1:B:59:ARG:HG3	1.82	0.61
1:A:508:ALA:HB2	1:A:671:ILE:HD11	1.82	0.60
1:B:121:LEU:HD22	1:B:134:VAL:CG2	2.30	0.60
1:B:392:ARG:HA	1:B:395:LEU:HD12	1.83	0.60
1:B:32:VAL:HG22	1:B:89:ARG:HB2	1.82	0.60
1:B:296:TRP:HE3	1:B:297:ILE:HD12	1.66	0.60
1:B:121:LEU:HD22	1:B:134:VAL:HG21	1.82	0.60
1:B:267:LEU:O	1:B:267:LEU:CD1	2.48	0.60
1:A:284:GLU:CD	1:A:284:GLU:H	2.03	0.60
1:B:475:VAL:HG13	1:B:543:LEU:HD23	1.84	0.60
1:A:238:GLY:HA2	1:A:259:GLY:HA3	1.83	0.60
1:B:144:GLY:HA3	1:B:177:MET:HE2	1.83	0.60
1:A:545:ARG:HH21	1:A:547:GLY:HA2	1.66	0.60
1:A:178:SER:O	1:A:179:LEU:C	2.41	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:GLN:H	1:A:516:GLN:CD	2.05	0.59
1:A:662:LEU:HD13	1:A:684:PHE:CD2	2.38	0.59
1:B:344:THR:HG22	1:B:345:ALA:H	1.67	0.59
1:A:486:ARG:HB3	1:A:515:PRO:HG3	1.84	0.59
1:A:136:ARG:NH1	1:A:296:TRP:CH2	2.71	0.59
1:A:327:VAL:HG23	1:A:332:ASP:HB2	1.82	0.59
1:A:342:GLN:CG	1:A:343:GLU:H	2.14	0.59
1:B:8:GLU:HG3	1:B:584:VAL:CG2	2.28	0.59
1:B:323:GLY:O	1:B:339:TYR:HA	2.03	0.59
1:A:28:ARG:HH21	1:A:93:LYS:HD3	1.66	0.59
1:A:549:VAL:HG23	1:A:550:PRO:HD2	1.84	0.59
1:B:14:PHE:HB3	1:B:306:PRO:HB2	1.83	0.59
1:B:103:PRO:CD	1:B:104:GLY:H	2.16	0.59
1:A:682:LEU:O	1:A:685:VAL:HG22	2.03	0.59
1:B:344:THR:HG23	1:B:404:GLN:HE21	1.68	0.59
1:B:485:PHE:HB2	1:B:553:GLU:OE1	2.03	0.59
1:A:184:ALA:HA	1:B:627:PRO:HG3	1.85	0.58
1:B:394:ALA:O	1:B:398:ALA:N	2.36	0.58
1:A:313:ALA:HB1	1:A:592:LEU:HD11	1.84	0.58
2:X:9:DT:C4	2:X:10:DA:N6	2.70	0.58
1:B:136:ARG:NH2	1:B:293:ILE:HG13	2.18	0.58
1:A:280:SER:HB2	2:C:7:DA:H5'	1.85	0.58
1:B:603:LEU:HG	1:B:605:THR:HG23	1.85	0.58
1:B:282:PRO:HG2	1:B:285:GLU:CB	2.33	0.58
1:B:344:THR:HG22	1:B:345:ALA:N	2.17	0.58
1:A:28:ARG:HD3	1:A:93:LYS:CE	2.34	0.58
1:A:645:SER:OG	1:A:646:GLY:N	2.36	0.58
1:B:365:LEU:O	1:B:368:ALA:HB3	2.04	0.58
1:B:310:ARG:HG3	1:B:310:ARG:HH11	1.69	0.57
1:B:580:ARG:NH2	2:X:7:DA:OP2	2.29	0.57
1:A:639:THR:HG22	1:A:640:ARG:NE	2.13	0.57
2:C:18:DT:O3'	2:C:19:DA:O4'	2.21	0.57
1:A:19:LEU:CD2	1:A:109:LEU:HD13	2.34	0.57
1:A:280:SER:HA	2:C:7:DA:H5'	1.85	0.57
1:A:300:ARG:HB3	1:A:300:ARG:NH1	2.19	0.57
1:A:449:ASN:HD21	2:C:2:DG:H21	1.53	0.57
1:B:455:LEU:HD22	1:B:460:LEU:HD22	1.86	0.57
1:A:445:HIS:NE2	3:H:18:C:O2'	2.37	0.57
1:B:596:LEU:O	1:B:597:GLU:C	2.41	0.57
1:B:114:ARG:HD3	1:B:132:LEU:CD1	2.24	0.57
1:A:11:LEU:C	1:A:13:ARG:H	2.09	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LEU:O	1:A:279:LEU:N	2.38	0.56
1:B:79:LEU:N	1:B:79:LEU:CD2	2.69	0.56
1:A:165:LEU:HD13	1:A:167:VAL:HG23	1.86	0.56
1:B:293:ILE:CD1	1:B:293:ILE:N	2.68	0.56
1:A:479:ALA:O	1:A:548:ARG:NH2	2.38	0.56
1:B:267:LEU:CD2	3:Y:12:C:O2'	2.54	0.56
1:B:504:THR:HG22	1:B:505:LEU:N	2.20	0.56
1:A:324:ARG:HD2	1:A:371:ALA:O	2.06	0.56
1:A:135:TYR:CZ	1:A:172:ARG:HB2	2.41	0.56
1:B:25:ARG:O	1:B:95:ARG:HD2	2.07	0.55
1:A:338:PHE:CZ	1:A:455:LEU:HD13	2.41	0.55
1:B:41:GLU:OE1	1:B:81:ARG:HD3	2.06	0.55
1:B:319:PRO:HG2	1:B:640:ARG:HD3	1.86	0.55
1:A:256:HIS:CE1	1:A:261:LEU:HD21	2.41	0.55
1:A:299:ARG:HG2	1:A:299:ARG:NH1	2.20	0.55
1:B:264:VAL:HG11	2:X:10:DA:P	2.47	0.55
1:A:329:LYS:HB2	1:A:646:GLY:O	2.07	0.55
1:B:99:ASP:OD2	1:B:101:LYS:HB2	2.07	0.55
1:B:60:MET:H	1:B:64:LEU:HA	1.72	0.55
1:B:314:TYR:O	1:B:592:LEU:HD12	2.06	0.55
1:A:138:GLU:CB	1:A:141:ARG:HH22	2.20	0.55
1:A:508:ALA:HB2	1:A:671:ILE:CD1	2.37	0.55
1:B:441:GLU:HG2	1:B:442:GLU:OE2	2.07	0.55
1:A:478:ASP:OD2	1:A:660:ASP:HA	2.06	0.55
1:A:607:HIS:O	1:A:608:ARG:O	2.25	0.55
2:X:2:DG:C2'	2:X:3:DA:O5'	2.55	0.55
3:Y:11:A:O2'	3:Y:12:C:H5'	2.07	0.55
1:A:324:ARG:HB3	1:A:336:VAL:O	2.06	0.54
2:C:2:DG:H2''	2:C:3:DA:O5'	2.06	0.54
1:A:445:HIS:CE1	3:H:18:C:H2'	2.42	0.54
1:A:312:GLN:HB2	6:A:693:HOH:O	2.06	0.54
1:A:593:TYR:CZ	1:A:595:PRO:HG3	2.42	0.54
1:A:32:VAL:HG22	1:A:89:ARG:HB2	1.88	0.54
1:A:288:ARG:O	1:A:292:GLU:HG3	2.08	0.54
1:B:437:VAL:CG1	1:B:438:PRO:CD	2.86	0.54
1:B:545:ARG:HG2	1:B:547:GLY:N	2.14	0.54
3:H:14:A:H2'	3:H:15:C:C6	2.42	0.54
1:A:138:GLU:CA	1:A:141:ARG:HH22	2.21	0.54
1:B:135:TYR:CE2	1:B:172:ARG:HB2	2.43	0.54
1:B:282:PRO:O	1:B:285:GLU:HB3	2.08	0.54
1:A:352:ASP:CB	1:A:437:VAL:HG21	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:TRP:HA	1:B:418:ARG:CB	2.38	0.53
3:H:11:A:C8	3:H:11:A:H3'	2.43	0.53
1:B:18:PRO:HA	1:B:162:ALA:CA	2.29	0.53
1:B:246:ASP:C	1:B:248:LYS:H	2.11	0.53
2:C:4:DG:H2'	2:C:5:DG:C8	2.43	0.53
1:A:17:ARG:HG2	1:A:18:PRO:N	2.22	0.53
1:A:190:PRO:HG2	1:A:263:PRO:HB3	1.89	0.53
1:A:575:LYS:N	3:H:9:U:OP1	2.41	0.53
1:A:76:GLU:CG	1:A:89:ARG:HG2	2.35	0.53
2:C:2:DG:H2''	2:C:3:DA:C5'	2.38	0.53
1:B:385:PRO:HA	1:B:391:PHE:CD1	2.44	0.53
1:B:603:LEU:HG	1:B:605:THR:CG2	2.38	0.53
1:A:200:ARG:HD2	1:A:202:TRP:CE2	2.44	0.53
1:A:350:ARG:CG	1:A:352:ASP:OD1	2.55	0.53
1:B:531:ARG:O	1:B:535:GLY:O	2.27	0.53
1:B:619:LEU:HD12	1:B:619:LEU:H	1.74	0.53
1:A:336:VAL:O	1:A:336:VAL:HG12	2.07	0.53
1:A:6:LYS:HG2	1:A:314:TYR:CE1	2.43	0.53
1:A:172:ARG:HD2	2:C:9:DT:OP1	2.08	0.53
1:B:344:THR:HG23	1:B:404:GLN:HG3	1.91	0.53
1:B:346:LEU:HD23	1:B:454:LEU:HD13	1.91	0.53
1:B:380:THR:HG22	1:B:381:LEU:N	2.24	0.53
1:A:411:PRO:HG3	1:A:437:VAL:CG1	2.38	0.53
1:B:102:ASP:HB3	1:B:105:GLU:HG2	1.90	0.53
1:B:142:GLY:HA3	1:B:145:TRP:CE2	2.45	0.53
1:B:434:ILE:HG21	2:X:1:DT:H1'	1.91	0.53
1:A:249:ASP:C	1:A:251:ARG:H	2.12	0.52
1:B:408:VAL:HB	1:B:434:ILE:HD13	1.92	0.52
3:H:13:U:O2'	3:H:14:A:H5'	2.09	0.52
3:H:17:U:O5'	3:H:18:C:OP2	2.26	0.52
3:Y:14:A:O2'	3:Y:15:C:H5'	2.10	0.52
1:A:176:GLU:OE1	1:A:176:GLU:N	2.37	0.52
1:A:280:SER:CA	2:C:7:DA:H5'	2.39	0.52
1:A:369:PHE:HB2	1:A:376:LEU:HD22	1.92	0.52
1:A:28:ARG:HD2	1:A:60:MET:HE1	1.92	0.52
1:B:223:LEU:O	1:B:226:TYR:HB3	2.10	0.52
3:H:13:U:H2'	3:H:14:A:H8	1.74	0.52
1:B:469:TYR:OH	1:B:637:HIS:HD2	1.92	0.52
1:A:33:LEU:CD1	1:A:37:PRO:HG2	2.40	0.52
1:B:98:LEU:HD23	1:B:109:LEU:HG	1.92	0.52
1:B:32:VAL:CG2	1:B:89:ARG:HB2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ASP:HB3	1:A:87:ALA:HB3	1.91	0.51
1:A:360:PHE:CD2	1:A:361:LEU:HD13	2.45	0.51
1:A:395:LEU:HD22	1:A:430:LEU:HD12	1.93	0.51
1:B:249:ASP:C	1:B:251:ARG:H	2.12	0.51
1:A:167:VAL:HG21	1:A:294:ALA:HB2	1.91	0.51
1:A:339:TYR:CD2	1:A:340:ARG:HD3	2.45	0.51
1:B:52:ARG:HG2	1:B:52:ARG:HH11	1.75	0.51
1:A:503:TRP:CE2	1:A:679:ARG:HA	2.45	0.51
1:B:462:VAL:HG12	1:B:463:VAL:HG13	1.93	0.51
1:A:449:ASN:ND2	2:C:2:DG:H21	2.09	0.51
1:B:4:LEU:HA	1:B:315:ARG:HB2	1.92	0.51
1:B:222:SER:HB3	1:B:225:ASP:HB2	1.91	0.51
1:B:551:GLN:O	1:B:553:GLU:N	2.44	0.51
1:A:12:ASN:HB2	1:A:167:VAL:O	2.10	0.51
1:A:327:VAL:HG22	1:A:328:SER:H	1.76	0.51
1:A:472:GLU:O	1:A:495:GLY:HA3	2.11	0.51
1:A:641:LEU:O	1:A:643:PRO:HD3	2.10	0.51
1:A:360:PHE:CE2	1:A:361:LEU:HD13	2.46	0.51
1:A:445:HIS:HE2	3:H:18:C:C2'	2.20	0.51
1:A:575:LYS:NZ	3:H:9:U:OP1	2.43	0.51
3:H:15:C:H2'	3:H:16:C:O4'	2.11	0.51
1:A:523:LEU:O	1:A:526:THR:HB	2.11	0.51
1:B:392:ARG:HA	1:B:395:LEU:CD1	2.41	0.51
1:B:437:VAL:O	1:B:439:LEU:N	2.44	0.51
1:B:524:GLU:C	1:B:526:THR:H	2.12	0.51
1:A:16:LEU:HB2	1:A:163:PHE:HB2	1.93	0.51
1:A:545:ARG:NH1	1:A:622:GLU:OE2	2.44	0.51
1:B:226:TYR:HE2	2:X:21:DT:H3'	1.75	0.51
1:B:236:ARG:HD2	1:B:260:LEU:CD2	2.41	0.51
1:A:32:VAL:CG1	1:A:91:TYR:HE1	2.24	0.50
1:A:76:GLU:HG2	1:A:89:ARG:CG	2.36	0.50
1:A:280:SER:O	1:A:281:LEU:HD23	2.10	0.50
1:A:342:GLN:HA	1:A:374:ALA:HB3	1.94	0.50
1:A:348:LEU:HD12	1:A:357:TRP:CE3	2.46	0.50
1:A:583:PRO:HB3	1:A:588:LEU:HG	1.92	0.50
1:B:25:ARG:HH11	1:B:25:ARG:HG2	1.76	0.50
1:B:437:VAL:HG13	1:B:438:PRO:CD	2.41	0.50
1:A:147:VAL:HG22	1:A:173:ILE:HG12	1.93	0.50
1:A:671:ILE:O	1:A:674:LEU:HG	2.11	0.50
1:A:110:SER:O	1:A:113:ALA:HB3	2.11	0.50
1:A:145:TRP:HZ2	1:A:271:HIS:O	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:PRO:O	1:B:540:ARG:HG2	2.12	0.50
1:A:482:ARG:O	1:A:548:ARG:HG2	2.11	0.50
1:A:573:VAL:HG22	1:A:619:LEU:HD23	1.92	0.50
1:B:192:ARG:CZ	2:X:10:DA:H4'	2.42	0.50
1:B:214:GLU:O	1:B:216:PRO:HD3	2.12	0.50
1:B:415:TRP:O	1:B:419:ASN:ND2	2.45	0.50
1:B:682:LEU:O	1:B:685:VAL:HG22	2.11	0.50
1:B:172:ARG:HG3	1:B:172:ARG:NH1	2.27	0.50
1:B:619:LEU:HD12	1:B:619:LEU:N	2.26	0.50
1:A:283:TRP:HZ3	1:A:287:ARG:NH1	2.10	0.50
1:A:300:ARG:HB3	1:A:300:ARG:CZ	2.41	0.50
1:B:593:TYR:CZ	1:B:595:PRO:HG3	2.47	0.50
1:B:501:LEU:CD1	1:B:682:LEU:HD11	2.30	0.50
3:H:16:C:O2'	3:H:17:U:H5'	2.12	0.50
1:A:443:GLU:OE2	1:A:446:ARG:NH2	2.45	0.49
1:A:583:PRO:HB3	1:A:588:LEU:CD2	2.42	0.49
1:B:122:ARG:HB3	1:B:122:ARG:HH11	1.77	0.49
1:B:318:ILE:N	1:B:318:ILE:HD12	2.27	0.49
1:B:636:PHE:O	1:B:639:THR:HB	2.12	0.49
1:A:149:GLY:HA2	1:A:171:TYR:CD1	2.47	0.49
1:A:175:CYS:SG	1:A:177:MET:HB3	2.52	0.49
1:A:296:TRP:O	1:A:299:ARG:HB3	2.12	0.49
1:B:213:LYS:O	1:B:213:LYS:HD3	2.11	0.49
1:B:370:GLY:C	1:B:372:SER:H	2.15	0.49
1:A:42:VAL:HG13	1:A:43:TYR:N	2.27	0.49
1:A:142:GLY:O	1:A:143:PRO:C	2.51	0.49
1:B:345:ALA:C	1:B:346:LEU:HD12	2.32	0.49
1:A:141:ARG:O	1:A:145:TRP:CH2	2.66	0.49
1:A:369:PHE:CB	1:A:376:LEU:HD22	2.43	0.49
3:H:11:A:C8	3:H:11:A:C3'	2.96	0.49
1:A:6:LYS:HE2	1:A:314:TYR:HE1	1.77	0.49
1:A:33:LEU:HD13	1:A:37:PRO:CG	2.42	0.49
1:B:110:SER:OG	1:B:156:TRP:HB2	2.12	0.49
1:B:168:ASP:OD2	1:B:580:ARG:NE	2.44	0.49
1:B:233:LEU:HD21	1:B:238:GLY:H	1.77	0.49
1:B:299:ARG:HG2	1:B:299:ARG:HH11	1.78	0.49
1:A:590:ASP:OD2	1:A:606:VAL:HA	2.12	0.49
1:B:156:TRP:CZ3	1:B:166:GLU:HB2	2.48	0.49
1:B:180:GLU:HG2	1:B:258:THR:CB	2.41	0.49
1:B:318:ILE:HD12	1:B:318:ILE:H	1.78	0.49
1:A:62:ASP:OD1	1:A:62:ASP:N	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:MET:HG3	1:B:181:ALA:CB	2.42	0.49
2:C:19:DA:H3'	2:C:20:DG:C5'	2.42	0.49
3:Y:15:C:H2'	3:Y:16:C:C6	2.48	0.48
1:A:348:LEU:HD23	1:A:348:LEU:C	2.33	0.48
2:C:20:DG:H2''	2:C:21:DT:O5'	2.13	0.48
1:B:453:GLY:O	1:B:457:LYS:HG3	2.13	0.48
3:Y:14:A:H2'	3:Y:15:C:O4'	2.12	0.48
1:A:155:LEU:HD23	1:A:164:LEU:O	2.13	0.48
1:B:207:LEU:HD13	1:B:240:ARG:NH1	2.28	0.48
1:A:344:THR:OG1	1:A:460:LEU:HD11	2.14	0.48
1:B:192:ARG:HD2	2:X:10:DA:H5''	1.94	0.48
1:B:638:LEU:HD23	1:B:641:LEU:HD12	1.96	0.48
1:A:327:VAL:CG2	1:A:328:SER:N	2.76	0.48
1:A:386:SER:C	1:A:388:GLY:H	2.17	0.48
1:B:386:SER:O	1:B:388:GLY:N	2.42	0.48
1:A:58:VAL:HG22	1:A:112:LEU:CD2	2.44	0.48
3:H:11:A:C5	3:H:12:C:C5	3.02	0.48
1:A:6:LYS:HE2	1:A:314:TYR:CE1	2.49	0.48
1:B:549:VAL:HG23	1:B:550:PRO:HD2	1.95	0.48
1:A:121:LEU:HD22	1:A:134:VAL:CG2	2.43	0.48
1:A:469:TYR:OH	1:A:637:HIS:HD2	1.97	0.48
1:B:144:GLY:HA3	1:B:177:MET:CE	2.42	0.48
1:B:192:ARG:HD2	2:X:10:DA:C5'	2.44	0.48
1:B:246:ASP:O	1:B:248:LYS:N	2.47	0.48
1:A:145:TRP:CZ2	1:A:269:ASP:CB	2.97	0.47
1:A:242:ALA:HB2	1:A:258:THR:HG22	1.96	0.47
1:B:654:ALA:HB3	1:B:655:PRO:HD3	1.95	0.47
1:A:369:PHE:CG	1:A:376:LEU:HD22	2.49	0.47
1:A:601:PHE:CE2	1:A:632:ALA:HB2	2.49	0.47
1:B:194:ARG:HG3	1:B:201:THR:HG22	1.96	0.47
1:B:516:GLN:OE1	1:B:553:GLU:HG2	2.14	0.47
1:B:486:ARG:CG	1:B:515:PRO:HD3	2.38	0.47
1:B:523:LEU:O	1:B:526:THR:HB	2.14	0.47
1:A:28:ARG:NH2	1:A:93:LYS:HD3	2.29	0.47
1:B:102:ASP:HB3	1:B:105:GLU:CG	2.45	0.47
1:A:242:ALA:HB2	1:A:258:THR:CG2	2.44	0.47
1:A:296:TRP:O	1:A:299:ARG:N	2.47	0.47
1:A:327:VAL:HG23	1:A:332:ASP:CB	2.43	0.47
1:A:384:HIS:ND1	1:A:385:PRO:HD2	2.30	0.47
1:B:134:VAL:O	1:B:150:GLY:HA3	2.15	0.47
1:B:195:ASN:OD1	1:B:256:HIS:HE1	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:SER:C	1:B:388:GLY:H	2.18	0.47
2:X:5:DG:C6	2:X:6:DT:O4	2.67	0.47
1:B:105:GLU:OE2	1:B:105:GLU:HA	2.15	0.47
1:B:319:PRO:HG3	1:B:637:HIS:ND1	2.30	0.47
1:A:11:LEU:C	1:A:13:ARG:N	2.68	0.47
1:A:346:LEU:HD23	1:A:454:LEU:HD22	1.97	0.47
1:A:654:ALA:HB3	1:A:655:PRO:HD3	1.96	0.47
1:B:173:ILE:HG22	2:X:9:DT:P	2.54	0.47
1:A:132:LEU:HD23	1:A:132:LEU:HA	1.71	0.47
1:B:102:ASP:CB	1:B:105:GLU:HG2	2.45	0.47
1:B:230:LYS:HB2	1:B:232:ARG:HD2	1.97	0.47
1:B:439:LEU:HD11	1:B:447:TRP:HD1	1.80	0.47
1:A:422:LYS:HE2	1:A:434:ILE:HD11	1.96	0.46
1:A:445:HIS:HA	1:A:647:PHE:CE2	2.51	0.46
1:B:270:LEU:O	1:B:271:HIS:CB	2.63	0.46
1:B:601:PHE:CE1	1:B:628:LEU:HD22	2.50	0.46
1:A:236:ARG:HD2	1:A:260:LEU:CD2	2.45	0.46
1:B:12:ASN:ND2	1:B:12:ASN:N	2.37	0.46
1:B:99:ASP:O	1:B:105:GLU:HB2	2.15	0.46
2:C:3:DA:C2'	2:C:4:DG:C8	2.98	0.46
1:A:141:ARG:HB2	1:A:274:GLU:CB	2.45	0.46
1:A:384:HIS:ND1	1:A:385:PRO:CD	2.79	0.46
1:B:545:ARG:C	1:B:547:GLY:H	2.19	0.46
1:B:150:GLY:O	1:B:169:PRO:HA	2.15	0.46
1:B:256:HIS:CD2	1:B:257:LEU:H	2.34	0.46
1:B:198:ASP:OD2	1:B:198:ASP:C	2.54	0.46
1:B:604:LEU:HD21	1:B:614:PRO:CB	2.40	0.46
1:A:230:LYS:HB2	1:A:232:ARG:HD2	1.98	0.46
1:A:251:ARG:O	1:A:253:PRO:HD3	2.16	0.46
1:B:359:GLU:O	1:B:363:ARG:HG2	2.15	0.46
1:B:435:LEU:HD13	1:B:450:ALA:CB	2.45	0.46
1:A:383:ALA:CB	1:A:391:PHE:HA	2.46	0.46
1:A:437:VAL:CG1	1:A:438:PRO:HD3	2.45	0.46
1:B:122:ARG:NH1	1:B:122:ARG:CB	2.79	0.46
1:B:448:GLU:HG2	1:B:647:PHE:HZ	1.80	0.46
1:A:33:LEU:HD12	1:A:37:PRO:HG2	1.98	0.46
1:B:171:TYR:O	2:X:8:DG:H5''	2.16	0.46
1:A:32:VAL:HG13	1:A:91:TYR:HE1	1.81	0.46
1:A:177:MET:HG3	1:A:181:ALA:HB3	1.97	0.46
1:A:469:TYR:HB3	1:A:470:PRO:CD	2.39	0.46
1:A:512:GLU:CD	1:A:512:GLU:N	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ARG:NH2	2:X:19:DA:N3	2.63	0.46
1:A:46:LEU:HB3	1:A:59:ARG:HG3	1.97	0.46
1:A:256:HIS:CD2	1:A:257:LEU:H	2.30	0.46
1:A:348:LEU:HB2	1:A:357:TRP:CZ2	2.51	0.46
1:A:440:ARG:C	1:A:442:GLU:H	2.19	0.46
1:B:310:ARG:HG3	1:B:310:ARG:NH1	2.30	0.46
1:B:532:ARG:C	1:B:534:ALA:N	2.70	0.46
1:B:666:VAL:HA	1:B:671:ILE:HG13	1.98	0.46
1:A:494:VAL:HG12	1:A:495:GLY:N	2.30	0.45
1:B:136:ARG:HH12	1:B:293:ILE:HG13	1.77	0.45
2:C:19:DA:H3'	2:C:20:DG:H5'	1.99	0.45
1:A:127:VAL:HG13	1:A:135:TYR:O	2.16	0.45
1:B:42:VAL:HG13	1:B:43:TYR:N	2.28	0.45
1:A:418:ARG:HD2	2:C:1:DT:H73	1.97	0.45
1:B:193:VAL:CG2	1:B:261:LEU:HB3	2.46	0.45
1:B:207:LEU:HD13	1:B:240:ARG:HH12	1.80	0.45
1:B:545:ARG:HD2	1:B:554:PHE:CE1	2.51	0.45
1:A:41:GLU:O	1:A:45:LEU:HG	2.17	0.45
1:A:190:PRO:HG2	1:A:263:PRO:CB	2.45	0.45
1:A:501:LEU:H	1:A:501:LEU:HD12	1.82	0.45
1:A:516:GLN:CB	1:A:556:LEU:HD23	2.42	0.45
1:B:43:TYR:N	1:B:44:PRO:CD	2.80	0.45
1:B:124:LEU:HD13	1:B:296:TRP:CH2	2.51	0.45
1:B:245:ALA:HB1	1:B:250:PRO:HA	1.99	0.45
1:A:28:ARG:CD	1:A:93:LYS:HE3	2.43	0.45
1:A:93:LYS:NZ	1:A:95:ARG:O	2.49	0.45
1:A:327:VAL:CG2	1:A:332:ASP:CB	2.87	0.45
1:A:395:LEU:HD22	1:A:430:LEU:CD1	2.47	0.45
1:A:590:ASP:N	1:A:607:HIS:NE2	2.65	0.45
1:B:102:ASP:CG	1:B:105:GLU:HG2	2.37	0.45
1:A:57:THR:HG22	1:A:66:SER:OG	2.17	0.45
1:B:549:VAL:CG2	1:B:550:PRO:HD2	2.46	0.45
1:A:527:LEU:HD23	1:A:527:LEU:HA	1.77	0.45
1:B:79:LEU:HD23	1:B:79:LEU:H	1.80	0.45
1:B:505:LEU:O	1:B:506:PRO:C	2.55	0.45
1:B:217:LEU:O	1:B:219:GLY:N	2.50	0.45
1:B:433:GLN:HB3	1:B:454:LEU:HG	1.98	0.45
1:B:642:TYR:HA	1:B:643:PRO:HD3	1.76	0.45
3:H:11:A:C2'	3:H:12:C:C5'	2.90	0.45
1:A:138:GLU:CB	1:A:141:ARG:NH2	2.76	0.45
1:A:325:ARG:HH11	1:A:325:ARG:CB	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:GLU:CG	1:B:584:VAL:HG21	2.35	0.45
1:A:469:TYR:CB	1:A:470:PRO:HD2	2.37	0.44
1:A:615:ARG:O	1:A:651:ARG:NH1	2.50	0.44
1:B:122:ARG:HH11	1:B:122:ARG:CB	2.30	0.44
1:A:315:ARG:HH11	1:A:315:ARG:HG2	1.82	0.44
1:B:29:LEU:HD22	1:B:90:LEU:HD13	1.98	0.44
1:A:69:PRO:O	1:A:72:VAL:HG22	2.17	0.44
1:B:524:GLU:C	1:B:526:THR:N	2.71	0.44
2:C:2:DG:C2'	2:C:3:DA:O5'	2.66	0.44
1:B:173:ILE:CG2	2:X:9:DT:OP1	2.57	0.44
1:B:446:ARG:HG3	2:X:2:DG:C8	2.52	0.44
2:C:9:DT:C4	2:C:10:DA:N6	2.86	0.44
1:A:165:LEU:HD13	1:A:167:VAL:CG2	2.48	0.44
1:A:346:LEU:CD2	1:A:454:LEU:HD13	2.40	0.44
1:A:433:GLN:NE2	1:A:434:ILE:O	2.49	0.44
1:B:7:THR:CG2	1:B:315:ARG:NH2	2.81	0.44
1:B:200:ARG:HD2	1:B:202:TRP:CZ2	2.53	0.44
1:A:596:LEU:O	1:A:597:GLU:C	2.55	0.44
1:A:28:ARG:HD2	1:A:60:MET:CE	2.48	0.44
1:A:139:HIS:HB3	1:A:147:VAL:O	2.17	0.44
1:B:32:VAL:HG23	1:B:32:VAL:O	2.16	0.44
1:B:103:PRO:CD	1:B:104:GLY:N	2.80	0.44
1:B:293:ILE:N	1:B:293:ILE:HD12	2.33	0.44
1:B:519:VAL:HG11	1:B:554:PHE:CD2	2.53	0.44
2:C:20:DG:C2'	2:C:21:DT:O5'	2.66	0.44
3:Y:15:C:N3	3:Y:16:C:C4	2.86	0.44
1:A:193:VAL:HG11	1:A:261:LEU:HD13	1.98	0.44
2:C:10:DA:C2'	2:C:11:DG:H5''	2.40	0.44
1:A:296:TRP:O	1:A:299:ARG:CB	2.65	0.43
1:A:531:ARG:O	1:A:535:GLY:N	2.49	0.43
1:B:267:LEU:HD21	3:Y:12:C:O2'	2.18	0.43
1:B:524:GLU:O	1:B:526:THR:N	2.51	0.43
1:A:34:ASP:O	1:A:87:ALA:N	2.49	0.43
1:A:42:VAL:O	1:A:45:LEU:HB2	2.18	0.43
1:A:45:LEU:O	1:A:48:GLN:N	2.47	0.43
1:A:284:GLU:CD	1:A:284:GLU:N	2.71	0.43
1:A:418:ARG:HG3	2:C:1:DT:C5	2.52	0.43
1:B:136:ARG:NH2	1:B:293:ILE:CG2	2.51	0.43
2:C:4:DG:H2'	2:C:5:DG:H8	1.83	0.43
1:A:422:LYS:NZ	1:A:432:SER:O	2.52	0.43
1:A:676:GLU:O	1:A:677:VAL:C	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:MET:H	1:A:64:LEU:HA	1.83	0.43
1:A:172:ARG:HG3	1:A:172:ARG:HH11	1.83	0.43
1:A:384:HIS:CG	1:A:385:PRO:HD2	2.53	0.43
1:A:400:GLU:C	1:A:402:GLY:H	2.22	0.43
1:A:449:ASN:OD1	1:A:645:SER:O	2.36	0.43
1:B:485:PHE:C	1:B:487:PHE:H	2.21	0.43
1:B:494:VAL:CG1	1:B:495:GLY:N	2.81	0.43
1:A:381:LEU:HD23	1:A:381:LEU:HA	1.76	0.43
1:B:223:LEU:HD11	1:B:257:LEU:HG	1.99	0.43
1:B:233:LEU:CD2	1:B:238:GLY:H	2.32	0.43
1:A:292:GLU:O	1:A:295:SER:N	2.52	0.43
1:B:41:GLU:C	1:B:44:PRO:HD2	2.39	0.43
1:B:327:VAL:HG21	1:B:332:ASP:HB2	1.96	0.43
1:B:457:LYS:HE2	1:B:685:VAL:HG23	2.00	0.43
1:B:672:ARG:HG3	1:B:672:ARG:NH1	2.32	0.43
1:A:309:VAL:O	1:A:309:VAL:CG2	2.67	0.43
1:A:503:TRP:CZ2	1:A:679:ARG:HA	2.54	0.43
1:B:210:GLU:OE2	1:B:243:TRP:HZ2	2.01	0.43
1:B:681:LYS:O	1:B:683:PHE:N	2.52	0.43
1:A:266:THR:O	1:A:267:LEU:C	2.56	0.43
1:A:517:GLU:O	1:A:521:ASP:HB2	2.19	0.43
1:A:594:VAL:HB	1:A:602:LEU:HB2	2.01	0.43
1:B:11:LEU:C	1:B:13:ARG:H	2.22	0.43
1:B:368:ALA:O	1:B:372:SER:HB3	2.19	0.43
1:A:79:LEU:N	1:A:79:LEU:HD23	2.33	0.43
1:A:252:LYS:CD	1:A:254:ILE:HD11	2.45	0.43
1:B:211:ASP:OD2	1:B:212:PRO:HD2	2.19	0.43
1:A:37:PRO:HB3	1:A:45:LEU:HD12	2.01	0.42
1:A:583:PRO:HD3	1:A:588:LEU:HD11	2.01	0.42
1:B:635:ILE:HG23	1:B:653:PRO:CG	2.49	0.42
1:A:292:GLU:O	1:A:293:ILE:C	2.57	0.42
1:B:100:PRO:O	1:B:159:ASP:OD1	2.37	0.42
1:B:280:SER:CB	2:X:7:DA:H5'	2.48	0.42
1:B:16:LEU:HB2	1:B:163:PHE:HB2	2.02	0.42
1:B:358:PRO:O	1:B:359:GLU:C	2.58	0.42
1:B:434:ILE:HB	2:X:1:DT:H4'	2.01	0.42
1:A:33:LEU:HD13	1:A:37:PRO:HG3	2.00	0.42
1:A:558:LEU:HD22	1:A:568:TYR:CD2	2.54	0.42
1:A:642:TYR:HA	1:A:643:PRO:HD3	1.85	0.42
3:H:11:A:N6	3:H:12:C:C4	2.87	0.42
1:A:115:ARG:HD2	1:A:115:ARG:HA	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:VAL:HG13	1:A:438:PRO:N	2.34	0.42
1:B:36:PRO:HA	1:B:37:PRO:HD3	1.81	0.42
1:B:117:LEU:HD23	1:B:132:LEU:HD22	2.02	0.42
1:B:178:SER:O	1:B:179:LEU:C	2.57	0.42
1:B:324:ARG:CB	1:B:336:VAL:HG12	2.49	0.42
1:B:601:PHE:CD1	1:B:628:LEU:HD22	2.55	0.42
3:Y:14:A:H2'	3:Y:15:C:H6	1.85	0.42
1:A:12:ASN:N	1:A:12:ASN:ND2	2.53	0.42
1:A:437:VAL:CG1	1:A:438:PRO:CD	2.98	0.42
1:B:19:LEU:N	1:B:19:LEU:HD12	2.35	0.42
2:C:9:DT:N3	2:C:10:DA:N6	2.68	0.42
1:A:102:ASP:HA	1:A:103:PRO:HD2	1.90	0.42
1:A:537:LEU:HD12	1:A:538:PRO:HD2	2.01	0.42
1:B:59:ARG:HA	1:B:64:LEU:HB3	2.02	0.42
1:B:215:LEU:C	1:B:215:LEU:HD13	2.39	0.42
1:A:98:LEU:HD12	1:A:98:LEU:HA	1.78	0.42
1:A:444:ARG:O	1:A:448:GLU:HB2	2.20	0.42
1:B:145:TRP:HE3	1:B:146:ARG:N	2.18	0.42
1:A:194:ARG:O	1:A:262:VAL:N	2.50	0.42
1:A:331:ALA:H	1:A:646:GLY:HA2	1.85	0.42
1:A:414:ALA:C	1:A:416:GLU:N	2.74	0.42
1:B:227:HIS:HE2	2:X:21:DT:HO3'	1.65	0.42
1:B:173:ILE:O	1:B:173:ILE:CG2	2.66	0.42
1:B:380:THR:CG2	1:B:381:LEU:N	2.83	0.42
1:B:394:ALA:HA	1:B:397:LYS:CB	2.50	0.42
1:A:102:ASP:O	1:A:103:PRO:C	2.58	0.41
1:A:272:GLU:CB	1:A:275:GLY:O	2.68	0.41
1:A:617:LEU:HD23	1:A:651:ARG:NH1	2.35	0.41
1:B:350:ARG:CZ	1:B:354:ALA:HB3	2.50	0.41
1:B:596:LEU:C	1:B:597:GLU:O	2.57	0.41
3:H:11:A:H3'	3:H:11:A:H8	1.84	0.41
1:A:58:VAL:O	1:A:64:LEU:HB2	2.20	0.41
1:A:318:ILE:HA	1:A:319:PRO:HD3	1.88	0.41
1:A:336:VAL:O	1:A:336:VAL:CG1	2.67	0.41
1:B:402:GLY:O	1:B:403:VAL:C	2.58	0.41
2:C:18:DT:O3'	2:C:19:DA:C4'	2.65	0.41
1:A:79:LEU:HG	1:A:86:TYR:HB2	2.03	0.41
1:A:372:SER:O	1:A:373:GLY:C	2.58	0.41
1:A:391:PHE:CE2	1:A:395:LEU:HD11	2.55	0.41
1:A:422:LYS:HE2	1:A:434:ILE:CD1	2.50	0.41
1:A:549:VAL:CG2	1:A:550:PRO:HD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:678:ASP:OD1	1:A:680:GLU:HB3	2.20	0.41
1:B:128:TRP:HE1	1:B:130:GLU:CD	2.23	0.41
1:B:376:LEU:HD11	1:B:378:LEU:HD21	2.03	0.41
2:C:4:DG:H1	3:H:16:C:H42	1.68	0.41
2:X:9:DT:C2'	2:X:10:DA:O5'	2.68	0.41
1:A:149:GLY:HA2	1:A:171:TYR:HD1	1.84	0.41
1:B:7:THR:HG23	1:B:315:ARG:NH2	2.35	0.41
1:A:348:LEU:HD23	1:A:349:LEU:N	2.36	0.41
1:A:437:VAL:HG13	1:A:438:PRO:HD3	2.01	0.41
1:A:546:ASP:O	1:A:548:ARG:N	2.53	0.41
1:B:135:TYR:CD2	1:B:172:ARG:HB2	2.56	0.41
1:B:344:THR:CG2	1:B:345:ALA:N	2.84	0.41
1:B:558:LEU:HD22	1:B:568:TYR:CD2	2.55	0.41
1:B:604:LEU:CD2	1:B:614:PRO:HB2	2.44	0.41
1:A:376:LEU:HD23	1:A:376:LEU:N	2.29	0.41
1:A:434:ILE:HG22	1:A:435:LEU:N	2.36	0.41
1:B:504:THR:CG2	1:B:505:LEU:N	2.83	0.41
3:Y:16:C:H2'	3:Y:17:U:C6	2.55	0.41
1:A:494:VAL:HG22	1:A:501:LEU:HB3	2.02	0.41
1:A:230:LYS:HB2	1:A:232:ARG:CD	2.51	0.41
1:A:327:VAL:CG2	1:A:328:SER:H	2.33	0.41
1:B:46:LEU:HD12	1:B:59:ARG:HD2	2.03	0.41
1:B:350:ARG:NH2	1:B:352:ASP:OD2	2.41	0.41
1:B:469:TYR:OH	1:B:637:HIS:CD2	2.72	0.41
1:B:531:ARG:O	1:B:531:ARG:HG2	2.19	0.41
1:B:546:ASP:O	1:B:548:ARG:N	2.53	0.41
1:B:554:PHE:O	1:B:558:LEU:HG	2.21	0.41
1:B:619:LEU:CD2	1:B:635:ILE:HD13	2.51	0.41
1:A:333:ALA:C	1:A:335:ARG:H	2.24	0.41
1:A:384:HIS:CE1	1:A:385:PRO:HG2	2.57	0.41
1:B:449:ASN:HD22	1:B:449:ASN:HA	1.51	0.41
1:A:117:LEU:HD23	1:A:132:LEU:HD22	2.03	0.40
1:A:299:ARG:NH1	1:A:299:ARG:CG	2.82	0.40
1:A:334:LEU:CD1	1:A:452:LEU:HD13	2.50	0.40
1:A:361:LEU:HD11	1:A:447:TRP:HB2	2.03	0.40
1:A:543:LEU:HB2	1:A:570:LEU:HD23	2.03	0.40
1:B:17:ARG:HD3	1:B:18:PRO:O	2.21	0.40
1:B:267:LEU:C	1:B:268:GLU:HG3	2.37	0.40
1:B:635:ILE:HG23	1:B:653:PRO:HG2	2.02	0.40
1:A:140:ALA:HB3	1:A:147:VAL:HB	2.02	0.40
1:A:215:LEU:HD12	1:A:223:LEU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:ILE:HD12	1:A:671:ILE:C	2.41	0.40
1:B:226:TYR:OH	2:X:21:DT:OP2	2.26	0.40
1:B:293:ILE:CD1	1:B:293:ILE:H	2.34	0.40
1:B:422:LYS:O	1:B:426:LEU:HB2	2.20	0.40
3:Y:11:A:C2'	3:Y:12:C:H5'	2.51	0.40
1:A:14:PHE:HA	1:A:307:GLU:O	2.21	0.40
1:A:635:ILE:HA	1:A:638:LEU:HD12	2.04	0.40
1:B:502:LEU:HD12	1:B:502:LEU:O	2.22	0.40
1:A:116:LEU:HD13	1:A:116:LEU:C	2.42	0.40
1:A:145:TRP:CZ2	1:A:271:HIS:O	2.72	0.40
1:B:168:ASP:OD1	1:B:169:PRO:HD2	2.21	0.40
1:A:389:LEU:HA	1:A:392:ARG:NH1	2.37	0.40
1:B:448:GLU:HB3	1:B:647:PHE:CZ	2.57	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ARG:NH1	1:B:234:GLN:O[2_755]	2.05	0.15
1:A:234:GLN:O	1:B:236:ARG:NH1[2_755]	2.18	0.02

## 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	
1	A	672/685 (98%)	577 (86%)	78 (12%)	17 (2%)	5	28
1	B	656/685 (96%)	545 (83%)	88 (13%)	23 (4%)	3	20
All	All	1328/1370 (97%)	1122 (84%)	166 (12%)	40 (3%)	4	24

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	PRO
1	A	675	LYS
1	B	143	PRO
1	B	387	GLN
1	B	547	GLY
1	B	552	ASP
1	A	278	ALA
1	A	373	GLY
1	A	598	ASP
1	A	682	LEU
1	B	94	GLY
1	B	96	ARG
1	B	97	PRO
1	B	238	GLY
1	B	239	GLY
1	B	374	ALA
1	B	403	VAL
1	B	682	LEU
1	A	107	SER
1	A	441	GLU
1	B	218	PRO
1	B	388	GLY
1	A	184	ALA
1	A	292	GLU
1	A	673	HIS
1	B	359	GLU
1	B	525	GLU
1	A	37	PRO
1	A	403	VAL
1	B	180	GLU
1	B	247	PRO
1	B	553	GLU
1	A	250	PRO
1	B	19	LEU
1	B	186	GLY
1	A	218	PRO
1	A	677	VAL
1	B	250	PRO
1	B	646	GLY
1	A	103	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	
1	A	471/549 (86%)	415 (88%)	56 (12%)	5	22
1	B	457/549 (83%)	409 (90%)	48 (10%)	7	27
All	All	928/1098 (84%)	824 (89%)	104 (11%)	6	24

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	29	LEU
1	A	62	ASP
1	A	64	LEU
1	A	93	LYS
1	A	130	GLU
1	A	136	ARG
1	A	141	ARG
1	A	143	PRO
1	A	155	LEU
1	A	160	SER
1	A	165	LEU
1	A	176	GLU
1	A	193	VAL
1	A	199	ARG
1	A	200	ARG
1	A	218	PRO
1	A	221	LEU
1	A	222	SER
1	A	223	LEU
1	A	232	ARG
1	A	233	LEU
1	A	234	GLN
1	A	284	GLU
1	A	286	ARG
1	A	288	ARG
1	A	299	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	300	ARG
1	A	309	VAL
1	A	340	ARG
1	A	343	GLU
1	A	361	LEU
1	A	366	LEU
1	A	396	ARG
1	A	400	GLU
1	A	452	LEU
1	A	454	LEU
1	A	462	VAL
1	A	472	GLU
1	A	500	HIS
1	A	501	LEU
1	A	507	GLU
1	A	516	GLN
1	A	521	ASP
1	A	524	GLU
1	A	528	TRP
1	A	532	ARG
1	A	570	LEU
1	A	575	LYS
1	A	580	ARG
1	A	590	ASP
1	A	597	GLU
1	A	600	THR
1	A	640	ARG
1	A	669	LEU
1	A	671	ILE
1	B	7	THR
1	B	12	ASN
1	B	17	ARG
1	B	52	ARG
1	B	57	THR
1	B	64	LEU
1	B	79	LEU
1	B	82	MET
1	B	95	ARG
1	B	119	GLU
1	B	120	ARG
1	B	137	ARG
1	B	143	PRO

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Mol	Chain	Res	Type
1	B	155	LEU
1	B	165	LEU
1	B	176	GLU
1	B	200	ARG
1	B	206	ARG
1	B	221	LEU
1	B	223	LEU
1	B	232	ARG
1	B	268	GLU
1	B	270	LEU
1	B	286	ARG
1	B	293	ILE
1	B	300	ARG
1	B	309	VAL
1	B	343	GLU
1	B	361	LEU
1	B	367	ARG
1	B	432	SER
1	B	441	GLU
1	B	449	ASN
1	B	454	LEU
1	B	501	LEU
1	B	516	GLN
1	B	540	ARG
1	B	541	VAL
1	B	545	ARG
1	B	546	ASP
1	B	552	ASP
1	B	580	ARG
1	B	590	ASP
1	B	600	THR
1	B	604	LEU
1	B	637	HIS
1	B	640	ARG
1	B	672	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	48	GLN
1	A	256	HIS

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Mol	Chain	Res	Type
1	A	449	ASN
1	A	461	GLN
1	A	551	GLN
1	A	637	HIS
1	B	12	ASN
1	B	48	GLN
1	B	256	HIS
1	B	404	GLN
1	B	436	ASN
1	B	449	ASN
1	B	621	HIS
1	B	637	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	H	10/20 (50%)	1 (10%)	0
3	Y	9/20 (45%)	2 (22%)	0
All	All	19/40 (47%)	3 (15%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	H	19	G
3	Y	11	A
3	Y	19	G

There are no RNA pucker outliers to report.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PO4	C	23	-	4,4,4	1.69	0	6,6,6	0.44	0

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, 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	A	677/685 (98%)	-0.44	2 (0%) 94 84	34, 67, 99, 111	3 (0%)
1	B	670/685 (97%)	-0.49	3 (0%) 92 79	37, 68, 100, 115	5 (0%)
2	C	16/21 (76%)	0.05	0 100 100	48, 74, 129, 134	0
2	X	15/21 (71%)	0.01	0 100 100	44, 57, 137, 148	0
3	H	12/20 (60%)	0.02	0 100 100	85, 103, 129, 130	0
3	Y	11/20 (55%)	0.13	0 100 100	91, 100, 134, 139	0
All	All	1401/1452 (96%)	-0.45	5 (0%) 92 79	34, 68, 101, 148	8 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	607	HIS	3.2
1	A	274	GLU	3.0
1	B	341	ALA	2.4
1	A	86	TYR	2.1
1	B	395	LEU	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
5	PO4	C	23	5/5	0.88	0.20	125,125,125,125	4
4	MG	X	22	1/1	0.94	0.22	47,47,47,47	0
4	MG	A	686	1/1	0.94	0.15	62,62,62,62	0
4	MG	C	22	1/1	0.97	0.17	39,39,39,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.