



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:36 PM GMT

PDB ID : 4M59  
Title : Crystal structure of the pentatricopeptide repeat protein PPR10 in complex with an 18-nt psaJ RNA element  
Authors : Yin, P.; Li, Q.; Yan, C.; Liu, Y.; Yan, N.  
Deposited on : 2013-08-08  
Resolution : 2.46 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

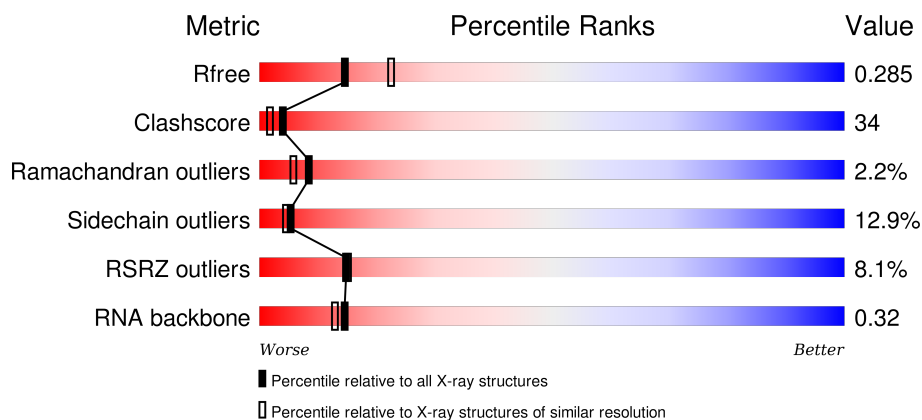
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.46 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	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)
RNA backbone	2183	1004 (2.92-2.00)

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 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	A	718	<div> <div>8%</div> <div>49%</div> <div>39%</div> <div>7%</div> <div>• • •</div> </div>
1	B	718	<div> <div>7%</div> <div>55%</div> <div>33%</div> <div>6%</div> <div>5%</div> </div>
2	C	18	<div> <div>6%</div> <div>39%</div> <div>17%</div> <div>22%</div> <div>22%</div> </div>
2	D	18	<div> <div>17%</div> <div>6%</div> <div>44%</div> <div>50%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11147 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 Chloroplast pentatricopeptide repeat protein 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	687	Total	C	N	O	S	0	0	0
			5202	3284	890	986	42			
1	B	683	Total	C	N	O	S	0	0	0
			5179	3273	891	974	41			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	256	SER	CYS	ENGINEERED MUTATION	UNP B8Y6I0
A	279	SER	CYS	ENGINEERED MUTATION	UNP B8Y6I0
A	430	SER	CYS	ENGINEERED MUTATION	UNP B8Y6I0
A	449	SER	CYS	ENGINEERED MUTATION	UNP B8Y6I0
B	256	SER	CYS	ENGINEERED MUTATION	UNP B8Y6I0
B	279	SER	CYS	ENGINEERED MUTATION	UNP B8Y6I0
B	430	SER	CYS	ENGINEERED MUTATION	UNP B8Y6I0
B	449	SER	CYS	ENGINEERED MUTATION	UNP B8Y6I0

- Molecule 2 is a RNA chain called psaJ RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	18	Total	C	N	O	P	0	0	0
			368	167	53	131	17			
2	C	14	Total	C	N	O	P	0	0	0
			279	126	41	99	13			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

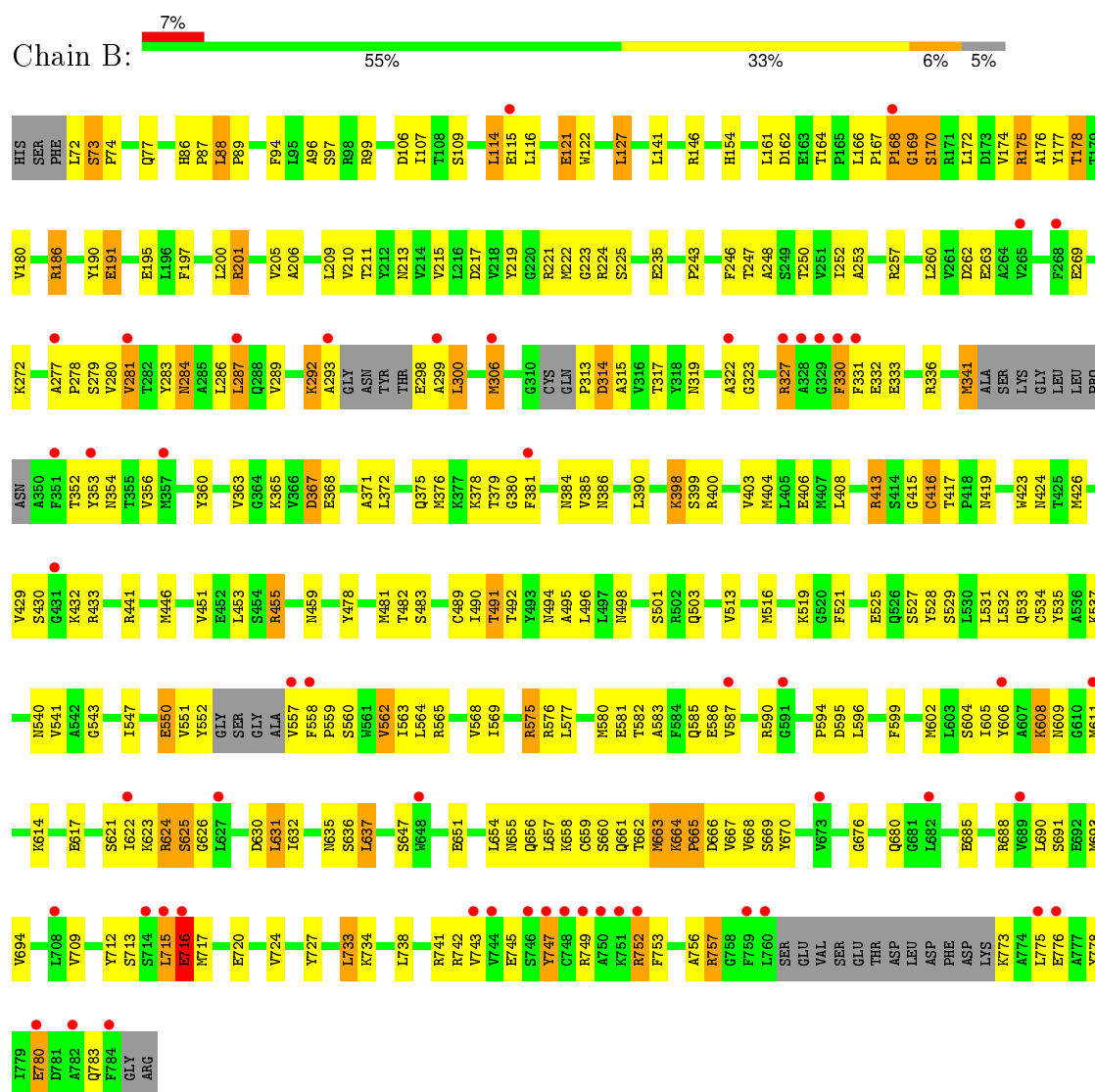


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total	O	0	0
			44	44		
4	B	59	Total	O	0	0
			59	59		
4	D	3	Total	O	0	0
			3	3		
4	C	8	Total	O	0	0
			8	8		

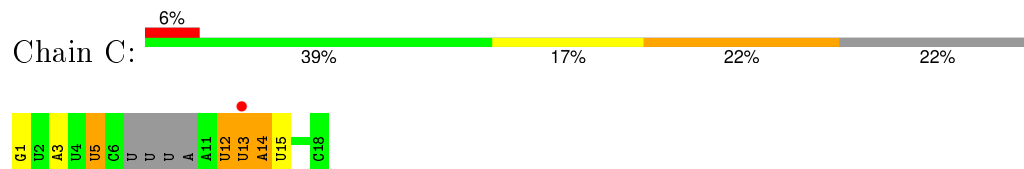




- Molecule 2: psaJ RNA



- Molecule 2: psaJ RNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.43Å 83.43Å 226.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.87 – 2.46 39.87 – 2.46	Depositor EDS
% Data completeness (in resolution range)	96.2 (39.87-2.46) 96.2 (39.87-2.46)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.07 (at 2.45Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, $R_{free}$	0.260 , 0.287 0.259 , 0.285	Depositor DCC
$R_{free}$ test set	2743 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.7	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 76.3	EDS
Estimated twinning fraction	0.065 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 54017 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11147	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.71	1/5294 (0.0%)	0.53	0/7177
1	B	0.77	0/5269	0.57	1/7136 (0.0%)
2	C	0.26	0/308	0.72	0/474
2	D	0.32	0/408	0.66	0/631
All	All	0.72	1/11279 (0.0%)	0.56	1/15418 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	468	CYS	CB-SG	-5.82	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	313	PRO	N-CA-CB	6.05	110.56	103.30

There are no chirality outliers.

There are no planarity outliers.

### 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	5202	0	5106	405	1
1	B	5179	0	5068	294	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	279	0	146	14	0
2	D	368	0	189	64	0
3	B	5	0	0	0	0
4	A	44	0	0	21	0
4	B	59	0	0	12	0
4	C	8	0	0	1	0
4	D	3	0	0	1	0
All	All	11147	0	10509	739	1

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 (739) 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:A:706:HIS:CE1	1:A:738:LEU:HD22	1.19	1.62
1:A:296:TYR:CE1	1:A:300:LEU:HD11	1.38	1.57
1:A:489:CYS:SG	1:A:491:THR:HG22	1.50	1.51
1:A:79:LEU:HD13	1:A:98:ARG:NH2	1.33	1.44
1:A:515:LYS:NZ	1:A:519:LYS:HE3	1.21	1.44
1:B:330:PHE:CE2	1:B:333:GLU:HG3	1.55	1.41
1:A:706:HIS:CE1	1:A:738:LEU:CD2	2.07	1.37
1:A:489:CYS:SG	1:A:491:THR:CG2	2.16	1.32
1:A:79:LEU:CD1	1:A:98:ARG:CZ	2.10	1.28
1:A:745:GLU:O	1:A:749:ARG:HG2	1.37	1.24
1:A:287:LEU:CD1	1:A:299:ALA:HB1	1.68	1.23
1:B:738:LEU:O	1:B:742:ARG:HG2	1.36	1.22
1:A:79:LEU:HD11	1:A:98:ARG:NE	1.56	1.20
1:A:515:LYS:NZ	1:A:519:LYS:CE	2.05	1.19
1:A:706:HIS:HE1	1:A:738:LEU:CD2	1.45	1.17
1:A:296:TYR:CD1	1:A:300:LEU:HD11	1.79	1.17
1:B:632:ILE:HD11	2:C:14:A:C2	1.80	1.16
2:D:5:U:H2'	2:D:6:C:H5''	1.24	1.14
1:B:552:TYR:OH	1:B:583:ALA:HB2	1.44	1.13
1:A:287:LEU:HD11	1:A:299:ALA:HB1	1.16	1.12
1:A:717:MET:HE3	1:A:720:GLU:OE1	1.46	1.12
1:A:740:TYR:O	1:A:743:VAL:HG22	1.47	1.12
1:A:128:ARG:NH2	1:A:163:GLU:HG2	1.63	1.11
2:D:9:U:H5'	2:D:10:A:OP2	1.52	1.10
1:B:599:PHE:HB3	1:B:622:ILE:HD11	1.23	1.10
1:A:296:TYR:CE1	1:A:300:LEU:CD1	2.33	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:GLN:HE22	1:A:708:LEU:HD21	1.12	1.07
1:B:279:SER:O	1:B:283:TYR:HD2	1.37	1.07
1:A:79:LEU:CD1	1:A:98:ARG:NH2	2.12	1.06
1:B:651:GLU:OE1	1:B:688:ARG:NH2	1.89	1.06
1:A:174:VAL:O	1:A:178:THR:HG23	1.56	1.05
1:B:559:PRO:HG2	1:B:590:ARG:NH2	1.71	1.05
2:D:9:U:H5''	2:D:10:A:H5'	1.35	1.05
1:A:128:ARG:HH21	1:A:163:GLU:HG2	0.90	1.04
1:A:717:MET:CE	1:A:720:GLU:OE1	2.03	1.04
1:A:128:ARG:HH21	1:A:163:GLU:CG	1.70	1.03
1:B:738:LEU:CD1	1:B:742:ARG:HD3	1.88	1.03
1:B:753:PHE:CD2	1:B:783:GLN:HG3	1.96	1.01
1:A:291:GLY:HA2	1:A:324:THR:HG23	1.43	1.00
1:A:715:LEU:O	1:A:717:MET:HG2	1.61	0.99
1:A:332:GLU:N	4:A:816:HOH:O	1.95	0.99
1:B:330:PHE:CD2	1:B:333:GLU:HG3	1.97	0.99
2:D:9:U:C5'	2:D:10:A:H5'	1.93	0.98
1:B:753:PHE:CE2	1:B:783:GLN:HA	1.98	0.98
1:B:547:ILE:O	1:B:551:VAL:HG23	1.62	0.98
1:B:175:ARG:HG2	2:D:1:G:N2	1.77	0.98
1:A:687:GLN:NE2	1:A:708:LEU:HD21	1.79	0.97
1:B:330:PHE:CE2	1:B:333:GLU:CG	2.48	0.97
1:A:79:LEU:HD11	1:A:98:ARG:CZ	1.85	0.97
1:B:599:PHE:HB3	1:B:622:ILE:CD1	1.95	0.96
1:B:175:ARG:HA	2:D:1:G:H21	1.28	0.96
1:B:552:TYR:HH	1:B:583:ALA:HB2	1.25	0.95
1:A:199:GLU:HG3	1:A:202:ARG:HH21	1.32	0.94
1:B:162:ASP:OD1	4:B:942:HOH:O	1.86	0.94
1:A:515:LYS:HZ3	1:A:519:LYS:CE	1.77	0.93
1:B:330:PHE:HE2	1:B:333:GLU:CG	1.82	0.92
1:A:548:GLU:OE1	1:A:576:ARG:NH2	2.02	0.92
1:A:296:TYR:HE1	1:A:300:LEU:HD11	1.15	0.92
1:A:86:HIS:NE2	1:A:90:THR:OG1	2.02	0.91
1:B:621:SER:HA	1:B:624:ARG:HG2	1.52	0.91
1:A:489:CYS:SG	1:A:491:THR:HG23	2.10	0.90
1:B:279:SER:O	1:B:283:TYR:CD2	2.25	0.90
1:B:283:TYR:HB3	1:B:306:MET:HG3	1.52	0.90
1:A:338:LEU:HD11	1:A:372:LEU:HG	1.54	0.90
1:A:291:GLY:CA	1:A:324:THR:HG23	2.01	0.90
1:A:515:LYS:HZ1	1:A:519:LYS:CE	1.75	0.89
2:D:5:U:C2'	2:D:6:C:H5''	2.01	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:TYR:OH	1:B:583:ALA:CB	2.20	0.89
2:D:9:U:C5'	2:D:10:A:OP2	2.19	0.89
1:A:651:GLU:OE1	1:A:688:ARG:NH2	2.03	0.89
1:B:559:PRO:HG2	1:B:590:ARG:HH21	1.32	0.89
1:B:632:ILE:CD1	2:C:14:A:C2	2.56	0.89
1:A:119:HIS:HD2	1:A:122:TRP:CZ3	1.91	0.89
1:B:594:PRO:HG2	1:B:599:PHE:CE2	2.07	0.89
1:A:296:TYR:OH	1:A:337:CYS:HB2	1.72	0.88
1:A:112:LYS:HD2	1:A:143:MET:CE	2.02	0.88
1:A:79:LEU:HD13	1:A:98:ARG:HH21	1.34	0.88
1:A:515:LYS:HZ3	1:A:519:LYS:HE3	1.32	0.88
1:B:738:LEU:HD12	1:B:742:ARG:HD3	1.52	0.88
1:A:295:ASN:OD1	1:A:298:GLU:HB2	1.74	0.88
1:A:79:LEU:HD13	1:A:98:ARG:CZ	1.87	0.88
1:A:175:ARG:HA	2:C:1:G:H21	1.38	0.87
1:A:287:LEU:CD1	1:A:299:ALA:CB	2.52	0.87
1:B:332:GLU:OE1	1:B:336:ARG:NH1	2.07	0.87
1:A:432:LYS:HG2	1:A:433:ARG:H	1.38	0.87
1:A:685:GLU:OE2	1:A:688:ARG:NH1	2.07	0.87
2:C:13:U:O2'	2:C:14:A:OP1	1.93	0.87
1:A:296:TYR:O	1:A:300:LEU:HG	1.75	0.86
1:B:660:SER:O	1:B:661:GLN:HB2	1.75	0.86
1:A:129:TRP:NE1	4:A:827:HOH:O	2.01	0.86
1:A:557:VAL:CG2	1:A:563:ILE:HD13	2.05	0.86
1:B:441:ARG:NH2	4:B:925:HOH:O	2.09	0.85
1:B:531:LEU:HD23	1:B:547:ILE:HD11	1.58	0.85
1:B:525:GLU:OE1	1:B:560:SER:OG	1.95	0.85
1:A:632:ILE:CD1	2:D:14:A:C2	2.58	0.85
1:B:664:LYS:O	1:B:665:PRO:O	1.95	0.85
1:A:296:TYR:CD1	1:A:300:LEU:CD1	2.56	0.85
1:B:175:ARG:HG2	2:D:1:G:C2	2.11	0.85
1:B:558:PHE:CE1	1:B:590:ARG:NH2	2.45	0.84
1:B:206:ALA:O	4:B:924:HOH:O	1.96	0.84
1:A:706:HIS:NE2	1:A:738:LEU:CD2	2.41	0.84
1:B:558:PHE:HE1	1:B:590:ARG:NH2	1.75	0.84
1:A:431:GLY:HA3	2:D:8:U:O2'	1.78	0.84
1:A:515:LYS:HZ3	1:A:519:LYS:CD	1.91	0.83
1:B:657:LEU:HD22	1:B:663:MET:HB3	1.60	0.83
1:A:106:ASP:HB3	1:A:109:SER:HB2	1.59	0.83
1:B:314:ASP:HA	1:B:317:THR:CG2	2.09	0.82
1:A:104:ARG:NH2	4:A:807:HOH:O	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:ASP:HA	1:B:317:THR:HG21	1.60	0.82
1:B:86:HIS:CD2	1:B:87:PRO:HD2	2.15	0.82
1:B:289:VAL:O	1:B:293:ALA:HB2	1.79	0.81
1:A:217:ASP:O	1:A:221:ARG:HG3	1.80	0.81
1:A:557:VAL:CG2	1:A:563:ILE:CD1	2.59	0.81
1:A:315:ALA:O	1:A:319:ASN:ND2	2.12	0.81
1:B:413:ARG:NH2	4:B:930:HOH:O	2.12	0.81
1:A:287:LEU:HD12	1:A:287:LEU:O	1.80	0.81
1:A:590:ARG:NH1	4:A:836:HOH:O	2.11	0.81
1:B:621:SER:O	1:B:625:SER:OG	1.98	0.81
1:A:717:MET:CB	1:A:720:GLU:OE1	2.29	0.81
1:A:710:GLY:C	2:D:18:C:O2'	2.19	0.79
2:D:6:C:H5'	2:D:6:C:H6	1.47	0.79
1:A:190:TYR:OH	4:A:801:HOH:O	1.99	0.79
1:A:489:CYS:HG	1:A:491:THR:HG22	1.44	0.79
1:A:83:ILE:HG23	1:A:91:LEU:HD11	1.64	0.79
1:A:717:MET:CE	1:A:720:GLU:CD	2.52	0.78
1:A:738:LEU:HD23	1:A:742:ARG:HD3	1.65	0.78
2:D:6:C:C5'	2:D:6:C:H6	1.95	0.78
1:B:558:PHE:HD1	1:B:559:PRO:HD2	1.47	0.78
2:C:13:U:HO2'	2:C:14:A:P	2.06	0.78
1:A:375:GLN:N	1:A:375:GLN:OE1	2.16	0.78
1:A:153:GLN:OE1	4:A:808:HOH:O	2.01	0.78
1:A:522:LYS:O	4:A:806:HOH:O	2.01	0.78
1:A:711:GLY:O	1:A:715:LEU:HB2	1.83	0.78
1:B:513:VAL:O	1:B:516:MET:HG2	1.84	0.78
1:B:738:LEU:O	1:B:742:ARG:CG	2.28	0.77
1:A:687:GLN:HB3	4:A:805:HOH:O	1.84	0.77
1:B:331:PHE:HZ	1:B:371:ALA:HB3	1.49	0.77
2:D:5:U:H2'	2:D:6:C:C5'	2.09	0.77
1:A:175:ARG:HA	2:C:1:G:N2	1.99	0.77
2:C:12:U:OP1	2:C:12:U:H4'	1.85	0.77
1:B:647:SER:OG	1:B:680:GLN:OE1	2.01	0.76
1:B:738:LEU:HD11	1:B:742:ARG:HD3	1.63	0.76
1:B:550:GLU:OE1	1:B:550:GLU:HA	1.86	0.76
1:A:316:VAL:HG23	2:C:5:U:C2	2.20	0.76
1:A:479:ASN:O	1:A:483:SER:OG	2.04	0.76
1:A:738:LEU:O	1:A:742:ARG:HG2	1.85	0.75
1:B:660:SER:OG	1:B:663:MET:HB2	1.86	0.75
1:A:548:GLU:HA	1:A:551:VAL:HG12	1.66	0.75
2:D:7:U:H5'	2:D:8:U:OP2	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:594:PRO:HG2	1:B:599:PHE:HE2	1.52	0.75
1:A:125:ALA:O	4:A:822:HOH:O	2.02	0.75
1:A:651:GLU:CD	1:A:688:ARG:NH2	2.39	0.75
1:A:706:HIS:NE2	1:A:738:LEU:HD22	1.92	0.74
1:B:551:VAL:HG13	1:B:557:VAL:O	1.86	0.74
1:A:717:MET:HB3	1:A:720:GLU:OE1	1.87	0.74
1:B:559:PRO:CG	1:B:590:ARG:NH2	2.49	0.74
1:A:354:ASN:O	1:A:358:THR:OG1	2.05	0.74
1:A:744:VAL:O	1:A:748:CYS:HB2	1.89	0.73
1:A:744:VAL:HB	1:A:779:ILE:HD11	1.69	0.73
1:A:112:LYS:HD2	1:A:143:MET:HE1	1.70	0.73
2:D:1:G:H3'	2:D:1:G:H8	1.53	0.73
1:B:210:VAL:HG21	2:D:1:G:C6	2.23	0.73
1:B:330:PHE:HE2	1:B:333:GLU:HG3	0.99	0.73
1:A:548:GLU:O	1:A:551:VAL:HG12	1.89	0.73
1:A:578:ASP:OD1	1:A:579:GLY:N	2.22	0.73
1:A:515:LYS:NZ	1:A:519:LYS:CD	2.52	0.73
2:C:13:U:H4'	2:C:14:A:OP2	1.87	0.73
2:D:5:U:O2'	2:D:6:C:OP1	2.03	0.73
1:B:314:ASP:CA	1:B:317:THR:CG2	2.67	0.72
1:A:112:LYS:HD2	1:A:143:MET:HE3	1.70	0.72
1:A:178:THR:HG21	1:A:211:THR:OG1	1.90	0.72
1:B:376:MET:HG2	1:B:381:PHE:CD2	2.24	0.72
1:A:661:GLN:OE1	1:B:384:ASN:OD1	2.08	0.72
1:B:341:MET:O	4:B:941:HOH:O	2.07	0.71
1:B:246:PHE:O	1:B:250:THR:OG1	2.06	0.71
1:B:558:PHE:CD1	1:B:559:PRO:HD2	2.23	0.71
2:D:9:U:C4'	2:D:10:A:OP2	2.38	0.71
1:A:104:ARG:CZ	4:A:807:HOH:O	2.39	0.71
1:B:280:VAL:O	1:B:284:ASN:ND2	2.24	0.71
1:A:477:MET:HE1	1:A:480:GLU:OE2	1.91	0.70
1:A:404:MET:HB3	1:A:426:MET:HE1	1.73	0.70
1:A:660:SER:OG	1:A:663:MET:O	2.09	0.70
1:B:753:PHE:CG	1:B:783:GLN:HG3	2.27	0.70
1:A:632:ILE:HD11	2:D:14:A:C2	2.26	0.70
1:A:717:MET:HB2	1:A:720:GLU:OE1	1.91	0.70
1:A:431:GLY:CA	2:D:8:U:O2'	2.40	0.69
1:A:296:TYR:CZ	1:A:300:LEU:HD21	2.28	0.69
1:A:662:THR:HG21	1:B:386:ASN:HB3	1.75	0.69
2:C:3:A:N7	4:C:107:HOH:O	2.26	0.69
1:A:106:ASP:CB	1:A:109:SER:HB2	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:ASP:O	1:A:669:SER:HB2	1.93	0.68
1:A:609:ASN:HB2	1:A:611:MET:HG3	1.76	0.68
1:A:717:MET:HE3	1:A:720:GLU:CD	2.11	0.68
1:A:283:TYR:OH	1:A:309:ASN:ND2	2.27	0.68
1:A:717:MET:HE2	1:A:720:GLU:HG3	1.75	0.68
1:A:565:ARG:NH1	4:A:826:HOH:O	1.92	0.68
1:A:565:ARG:NH2	1:A:595:ASP:OD2	2.26	0.68
1:B:314:ASP:C	1:B:317:THR:CG2	2.62	0.68
1:A:341:MET:CE	1:A:348:PRO:HG3	2.24	0.68
1:A:705:TYR:O	1:A:709:VAL:HG23	1.93	0.68
2:D:1:G:C8	2:D:1:G:H3'	2.30	0.67
1:B:209:LEU:O	1:B:213:ASN:ND2	2.27	0.67
1:A:456:ASP:O	1:A:460:THR:HG23	1.95	0.67
1:A:200:LEU:HD23	1:A:200:LEU:C	2.15	0.67
1:B:88:LEU:N	1:B:89:PRO:HD2	2.10	0.67
2:D:14:A:O2'	2:D:15:U:OP1	2.13	0.67
1:A:284:ASN:O	1:A:320:GLU:OE1	2.13	0.67
1:B:491:THR:OG1	4:B:928:HOH:O	2.12	0.67
1:A:717:MET:HE2	1:A:720:GLU:CD	2.15	0.67
1:A:701:CYS:HG	1:A:704:THR:HG1	1.41	0.66
1:A:498:ASN:O	1:A:501:SER:OG	2.08	0.66
1:B:376:MET:CE	1:B:381:PHE:CE2	2.78	0.66
1:B:269:GLU:HA	1:B:272:LYS:HD2	1.77	0.66
1:A:760:LEU:HD12	1:A:760:LEU:C	2.16	0.66
1:B:577:LEU:HD21	1:B:611:MET:CE	2.26	0.66
1:B:651:GLU:CD	1:B:688:ARG:NH2	2.50	0.66
1:B:190:TYR:OH	4:B:927:HOH:O	1.97	0.65
1:A:150:ARG:HH11	1:A:150:ARG:HG2	1.61	0.65
2:D:12:U:H6	2:D:12:U:O5'	1.79	0.65
1:A:631:LEU:HD13	1:A:666:ASP:HB2	1.79	0.65
1:A:419:ASN:H	1:A:419:ASN:HD22	1.44	0.65
1:B:757:ARG:NH2	1:B:783:GLN:OE1	2.26	0.65
1:A:447:ARG:HH22	1:A:477:MET:HE1	1.61	0.65
1:A:721:ALA:O	1:A:725:ILE:HG13	1.97	0.65
1:B:174:VAL:O	1:B:178:THR:HG23	1.96	0.65
2:C:12:U:C5	2:C:14:A:C2	2.85	0.64
2:D:9:U:H5'	2:D:10:A:H5'	1.78	0.64
2:D:9:U:H5''	2:D:10:A:C5'	2.18	0.64
1:B:175:ARG:HA	2:D:1:G:N2	2.06	0.64
1:A:651:GLU:OE2	1:A:688:ARG:NH2	2.30	0.64
1:A:338:LEU:HD11	1:A:372:LEU:CG	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:MET:HG2	1:A:369:ALA:HB1	1.79	0.64
1:B:565:ARG:NH2	1:B:595:ASP:OD2	2.30	0.64
1:A:111:LEU:HD13	1:A:144:VAL:HG23	1.79	0.64
1:A:338:LEU:HD22	1:A:375:GLN:HG2	1.80	0.64
1:B:260:LEU:HB3	1:B:263:GLU:HG2	1.79	0.64
1:A:740:TYR:C	1:A:743:VAL:HG22	2.18	0.64
1:A:353:TYR:OH	4:A:825:HOH:O	2.13	0.64
1:A:532:LEU:HD13	1:A:547:ILE:HD12	1.80	0.64
1:A:738:LEU:CD2	1:A:742:ARG:HD3	2.28	0.63
1:B:559:PRO:HD2	1:B:590:ARG:HH22	1.63	0.63
1:B:666:ASP:O	1:B:669:SER:N	2.32	0.63
1:A:706:HIS:NE2	1:A:738:LEU:HD23	2.13	0.63
1:A:717:MET:HE2	1:A:720:GLU:OE1	1.92	0.63
1:A:163:GLU:HG3	1:A:164:THR:N	2.13	0.63
1:A:760:LEU:HD22	1:A:779:ILE:HG13	1.79	0.63
1:B:583:ALA:O	1:B:587:VAL:HG23	1.99	0.63
1:A:178:THR:CG2	1:A:211:THR:OG1	2.46	0.63
1:A:634:TYR:O	1:A:638:MET:HG3	1.98	0.63
1:A:419:ASN:ND2	1:A:422:THR:H	1.96	0.63
1:B:494:ASN:OD1	1:B:527:SER:OG	2.15	0.63
1:A:743:VAL:O	1:A:747:TYR:HB2	1.97	0.63
1:A:257:ARG:NH1	4:A:804:HOH:O	2.30	0.63
1:B:651:GLU:CD	1:B:688:ARG:HH22	2.03	0.63
1:B:481:MET:HE1	1:B:492:THR:HG21	1.80	0.63
1:A:142:GLU:HG3	1:A:172:LEU:HD23	1.81	0.62
1:A:543:GLY:O	1:A:547:ILE:HG13	2.00	0.62
1:A:338:LEU:CD2	1:A:375:GLN:CB	2.78	0.62
1:A:717:MET:HE2	1:A:720:GLU:CG	2.30	0.62
1:A:740:TYR:O	1:A:743:VAL:CG2	2.36	0.62
1:B:379:THR:OG1	1:B:379:THR:O	2.12	0.62
1:A:419:ASN:ND2	1:A:419:ASN:H	1.98	0.61
1:A:260:LEU:HB3	1:A:263:GLU:CG	2.29	0.61
1:A:515:LYS:HZ1	1:A:519:LYS:HE3	0.79	0.61
1:A:552:TYR:HE1	1:A:586:GLU:HG3	1.66	0.61
1:B:657:LEU:HD22	1:B:663:MET:CB	2.29	0.61
1:B:174:VAL:HG22	1:B:205:VAL:CG1	2.30	0.61
1:A:147:ALA:O	1:A:151:GLU:N	2.34	0.61
1:A:516:MET:O	1:A:521:PHE:HB2	2.00	0.61
1:A:401:PHE:HE1	1:A:429:VAL:HG21	1.64	0.61
1:B:757:ARG:NH2	1:B:780:GLU:OE1	2.33	0.61
1:B:201:ARG:NH2	1:B:235:GLU:OE1	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:ARG:NH1	2:D:18:C:C2	2.68	0.61
1:A:287:LEU:HD13	1:A:299:ALA:HB1	1.79	0.61
1:A:557:VAL:HG21	1:A:563:ILE:HD13	1.81	0.61
1:A:246:PHE:O	1:A:250:THR:OG1	2.14	0.61
1:B:717:MET:O	1:B:720:GLU:HG2	2.01	0.61
1:A:557:VAL:HG23	1:A:563:ILE:CD1	2.31	0.60
1:A:407:MET:O	1:A:411:MET:HG3	2.01	0.60
1:B:595:ASP:OD1	1:B:595:ASP:N	2.25	0.60
1:A:548:GLU:CA	1:A:551:VAL:HG12	2.31	0.60
1:A:477:MET:CE	1:A:480:GLU:OE2	2.49	0.60
1:A:745:GLU:HA	1:A:778:TYR:OH	2.01	0.60
1:A:419:ASN:ND2	1:A:422:THR:OG1	2.34	0.60
1:B:73:SER:O	1:B:77:GLN:HG3	2.02	0.60
1:A:119:HIS:CD2	1:A:122:TRP:CZ3	2.81	0.60
1:A:660:SER:O	1:A:662:THR:HG22	2.02	0.60
1:A:489:CYS:SG	1:A:490:ILE:N	2.75	0.59
1:A:98:ARG:HH21	1:A:101:GLU:CD	2.05	0.59
1:B:654:LEU:HD23	1:B:658:LYS:HE3	1.84	0.59
1:A:700:PRO:HB3	1:A:704:THR:HG21	1.82	0.59
1:A:366:VAL:HG12	1:A:394:MET:HE3	1.83	0.59
1:A:432:LYS:HG2	1:A:433:ARG:N	2.14	0.59
1:A:447:ARG:NH2	1:A:477:MET:HE1	2.17	0.59
1:B:630:ASP:OD1	1:B:631:LEU:N	2.35	0.59
1:B:168:PRO:O	1:B:169:GLY:O	2.21	0.59
1:A:757:ARG:O	1:A:760:LEU:HG	2.03	0.59
1:A:219:TYR:CE1	1:A:228:ARG:HD2	2.37	0.59
1:B:540:ASN:OD1	1:B:543:GLY:N	2.33	0.59
1:A:111:LEU:HD13	1:A:144:VAL:CG2	2.33	0.59
1:A:349:ASN:N	1:A:349:ASN:OD1	2.33	0.59
1:A:446:MET:O	1:A:451:VAL:HG12	2.02	0.59
1:A:548:GLU:HA	1:A:551:VAL:CG1	2.33	0.59
1:B:289:VAL:O	1:B:293:ALA:CB	2.49	0.59
1:A:284:ASN:ND2	1:A:316:VAL:HG13	2.18	0.58
1:B:575:ARG:CD	1:B:605:ILE:HD13	2.33	0.58
1:A:260:LEU:HB3	1:A:263:GLU:HG3	1.85	0.58
1:B:94:PHE:O	1:B:97:SER:OG	2.18	0.58
1:A:711:GLY:N	2:D:18:C:O2'	2.36	0.58
1:B:284:ASN:N	1:B:284:ASN:HD22	2.01	0.58
1:A:742:ARG:NH1	2:D:18:C:N1	2.52	0.58
2:D:1:G:C8	2:D:1:G:C3'	2.86	0.58
1:A:745:GLU:O	1:A:749:ARG:CG	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:TYR:O	1:A:300:LEU:CG	2.49	0.58
1:B:577:LEU:HD13	1:B:605:ILE:HG13	1.84	0.58
1:A:79:LEU:HD11	1:A:98:ARG:HE	1.63	0.57
1:A:489:CYS:SG	1:A:491:THR:N	2.76	0.57
1:A:675:ASN:ND2	2:D:17:U:H5''	2.19	0.57
1:A:660:SER:C	1:A:662:THR:H	2.08	0.57
1:A:565:ARG:NE	4:A:826:HOH:O	2.35	0.57
1:B:459:ASN:OD1	1:B:492:THR:HG22	2.03	0.57
1:B:262:ASP:CG	4:B:919:HOH:O	2.42	0.57
1:A:519:LYS:HB3	1:A:521:PHE:CD2	2.39	0.57
1:B:560:SER:OG	1:B:562:VAL:HG23	2.04	0.57
1:A:712:TYR:O	1:A:717:MET:O	2.22	0.57
1:A:86:HIS:CD2	1:A:87:PRO:O	2.57	0.57
1:B:376:MET:HE1	1:B:381:PHE:CE2	2.38	0.57
1:A:738:LEU:O	1:A:742:ARG:CG	2.51	0.57
1:B:660:SER:C	1:B:662:THR:H	2.09	0.56
1:A:296:TYR:HH	1:A:337:CYS:HB2	1.71	0.56
1:A:744:VAL:HG23	1:A:745:GLU:N	2.20	0.56
1:A:353:TYR:HE2	1:A:381:PHE:HD2	1.54	0.56
1:A:631:LEU:CD1	1:A:666:ASP:HB2	2.34	0.56
1:A:429:VAL:O	1:A:467:ARG:NH1	2.30	0.56
1:B:666:ASP:O	1:B:668:VAL:N	2.38	0.56
1:B:292:LYS:HA	1:B:327:ARG:HD3	1.86	0.56
1:B:459:ASN:CG	1:B:492:THR:HG22	2.27	0.56
1:A:200:LEU:HD23	1:A:201:ARG:N	2.21	0.56
1:A:753:PHE:O	1:A:756:ALA:HB3	2.06	0.55
2:D:9:U:H4'	2:D:10:A:OP2	2.05	0.55
1:A:86:HIS:HD2	1:A:87:PRO:O	1.90	0.55
1:A:296:TYR:HE1	1:A:300:LEU:CD1	2.00	0.55
1:B:86:HIS:CD2	1:B:87:PRO:CD	2.89	0.55
1:B:657:LEU:CD2	1:B:663:MET:HG3	2.37	0.55
1:A:519:LYS:HB3	1:A:521:PHE:CE2	2.41	0.55
1:B:314:ASP:C	1:B:317:THR:HG22	2.25	0.55
1:B:330:PHE:CD2	1:B:333:GLU:CG	2.81	0.55
1:A:231:ALA:O	1:A:235:GLU:HG3	2.07	0.55
1:A:174:VAL:O	1:A:178:THR:CG2	2.45	0.55
1:B:660:SER:O	1:B:661:GLN:CB	2.49	0.55
1:B:178:THR:HG21	1:B:211:THR:OG1	2.07	0.55
1:B:114:LEU:HD22	1:B:122:TRP:HB3	1.88	0.55
1:B:599:PHE:CD1	1:B:622:ILE:HG12	2.42	0.55
1:A:377:LYS:C	1:A:379:THR:H	2.09	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:773:LYS:N	1:B:776:GLU:OE1	2.39	0.55
1:B:594:PRO:HG2	1:B:599:PHE:CZ	2.41	0.55
1:A:432:LYS:CG	1:A:433:ARG:H	2.16	0.55
1:A:571:ASN:HB3	1:A:580:MET:HG3	1.89	0.55
1:B:580:MET:HG2	1:B:602:MET:HE2	1.89	0.55
1:A:270:ASP:O	1:A:274:ARG:HG3	2.07	0.55
1:A:284:ASN:ND2	1:A:316:VAL:CG1	2.70	0.54
1:A:280:VAL:HG23	1:A:281:VAL:H	1.71	0.54
1:B:367:ASP:OD2	1:B:400:ARG:NH1	2.38	0.54
1:A:431:GLY:N	2:D:8:U:O2'	2.40	0.54
1:B:666:ASP:O	1:B:667:VAL:C	2.45	0.54
1:A:754:GLU:HA	1:A:757:ARG:HE	1.71	0.54
1:A:731:HIS:HA	4:A:834:HOH:O	2.08	0.54
1:A:608:LYS:HG3	4:A:841:HOH:O	2.07	0.54
1:A:340:THR:C	1:A:342:ALA:H	2.09	0.54
1:A:128:ARG:NE	1:A:163:GLU:OE1	2.32	0.54
1:A:353:TYR:HE2	1:A:381:PHE:CD2	2.26	0.54
1:B:306:MET:HE1	1:B:317:THR:HG21	1.90	0.54
1:A:272:LYS:NZ	1:A:305:GLU:OE1	2.40	0.54
1:A:709:VAL:O	1:A:713:SER:N	2.41	0.54
1:B:167:PRO:HB2	1:B:168:PRO:HD2	1.88	0.54
1:A:286:LEU:HD12	1:A:286:LEU:O	2.07	0.54
1:A:76:ALA:O	1:A:79:LEU:N	2.40	0.54
1:B:577:LEU:HD21	1:B:611:MET:HE1	1.88	0.54
1:A:632:ILE:HD13	2:D:14:A:C2	2.42	0.54
1:A:504:GLY:O	1:A:506:TRP:N	2.41	0.54
1:A:174:VAL:HG21	1:A:208:THR:HG23	1.89	0.54
1:A:582:THR:O	1:A:585:GLN:HB3	2.08	0.54
1:A:742:ARG:NH1	2:D:18:C:C6	2.76	0.53
1:A:668:VAL:O	1:A:672:THR:OG1	2.17	0.53
1:A:715:LEU:C	1:A:717:MET:HG2	2.27	0.53
1:A:718:PHE:CD1	1:A:747:TYR:CE1	2.96	0.53
1:B:279:SER:OG	1:B:280:VAL:N	2.42	0.53
1:A:745:GLU:HA	1:A:778:TYR:CZ	2.43	0.53
1:B:586:GLU:O	1:B:590:ARG:HG3	2.08	0.53
1:B:174:VAL:HG22	1:B:205:VAL:HG12	1.90	0.53
1:B:709:VAL:O	1:B:713:SER:OG	2.25	0.53
1:B:596:LEU:HD21	1:B:630:ASP:HB2	1.90	0.53
1:A:718:PHE:CG	1:A:747:TYR:CE1	2.97	0.53
1:A:399:SER:OG	1:A:432:LYS:HE3	2.08	0.53
1:A:353:TYR:CE2	1:A:381:PHE:HD2	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:ARG:CG	2:D:1:G:N2	2.63	0.52
1:B:724:VAL:O	1:B:727:TYR:N	2.43	0.52
1:A:79:LEU:CD1	1:A:98:ARG:NE	2.34	0.52
2:D:7:U:O2	2:D:7:U:H2'	2.09	0.52
2:D:13:U:H3'	2:D:13:U:H6	1.75	0.52
1:A:754:GLU:C	1:A:756:ALA:H	2.12	0.52
1:B:715:LEU:O	1:B:716:GLU:C	2.48	0.52
1:A:698:MET:O	1:A:700:PRO:HD3	2.09	0.52
1:B:577:LEU:HD22	1:B:609:ASN:HD22	1.73	0.52
1:A:460:THR:OG1	1:A:461:LEU:N	2.42	0.52
1:A:419:ASN:ND2	1:A:419:ASN:N	2.55	0.52
1:B:408:LEU:HD13	1:B:426:MET:SD	2.49	0.52
1:B:376:MET:HE1	1:B:381:PHE:CZ	2.45	0.51
1:A:725:ILE:C	1:A:727:TYR:H	2.12	0.51
1:B:88:LEU:N	1:B:89:PRO:CD	2.72	0.51
1:A:739:THR:O	1:A:742:ARG:HG2	2.11	0.51
1:A:88:LEU:HB3	1:A:89:PRO:HD3	1.92	0.51
1:B:298:GLU:C	1:B:300:LEU:H	2.12	0.51
1:B:432:LYS:HG2	1:B:433:ARG:H	1.75	0.51
1:B:379:THR:O	1:B:381:PHE:N	2.36	0.51
1:A:150:ARG:NH1	1:A:150:ARG:HG2	2.24	0.51
2:D:5:U:C3'	2:D:6:C:H5''	2.40	0.51
1:B:166:LEU:HD13	1:B:170:SER:HB3	1.92	0.51
1:B:253:ALA:O	1:B:257:ARG:HG3	2.11	0.51
1:B:575:ARG:HD2	1:B:605:ILE:HD13	1.93	0.51
2:C:13:U:OP1	2:C:13:U:H3'	2.11	0.51
1:B:657:LEU:CD2	1:B:663:MET:CB	2.88	0.51
2:D:12:U:H4'	2:D:14:A:H5''	1.94	0.51
1:A:456:ASP:O	1:A:460:THR:CG2	2.59	0.51
1:B:602:MET:O	1:B:605:ILE:HG22	2.10	0.51
1:B:631:LEU:O	1:B:635:ASN:N	2.41	0.51
1:A:668:VAL:HG13	2:D:16:U:C2	2.46	0.51
1:A:683:VAL:HB	1:A:712:TYR:CE1	2.46	0.50
1:A:221:ARG:NH1	1:B:433:ARG:HD3	2.27	0.50
1:B:419:ASN:ND2	4:B:945:HOH:O	2.27	0.50
1:B:552:TYR:OH	1:B:583:ALA:CA	2.59	0.50
1:B:685:GLU:OE1	1:B:688:ARG:NH1	2.44	0.50
1:A:661:GLN:O	1:B:354:ASN:ND2	2.44	0.50
1:A:510:GLN:O	1:A:512:ILE:N	2.44	0.50
1:B:564:LEU:O	1:B:568:VAL:HG23	2.11	0.50
1:A:291:GLY:HA2	1:A:324:THR:CG2	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:GLU:C	1:A:551:VAL:HG12	2.32	0.50
1:A:119:HIS:HD2	1:A:122:TRP:CE3	2.28	0.50
1:B:635:ASN:ND2	1:B:669:SER:OG	2.30	0.50
1:B:323:GLY:O	1:B:327:ARG:HG2	2.11	0.50
1:A:753:PHE:O	1:A:756:ALA:N	2.43	0.50
1:A:740:TYR:HA	1:A:743:VAL:HG22	1.94	0.50
1:A:586:GLU:O	1:A:590:ARG:N	2.30	0.50
1:B:599:PHE:CB	1:B:622:ILE:HD11	2.17	0.50
1:B:528:TYR:O	1:B:532:LEU:HD13	2.12	0.50
1:B:599:PHE:CG	1:B:622:ILE:HG12	2.47	0.49
1:B:217:ASP:O	1:B:221:ARG:HG3	2.12	0.49
1:B:712:TYR:HD1	1:B:717:MET:SD	2.35	0.49
1:B:690:LEU:O	1:B:694:VAL:HG23	2.12	0.49
1:B:423:TRP:CD2	1:B:446:MET:HG3	2.47	0.49
1:B:688:ARG:O	1:B:691:SER:OG	2.26	0.49
1:A:775:LEU:O	1:A:777:ALA:N	2.46	0.49
1:B:529:SER:O	1:B:533:GLN:HG3	2.12	0.49
1:A:371:ALA:O	1:A:375:GLN:OE1	2.29	0.49
1:A:443:LEU:HD22	1:A:461:LEU:HD22	1.95	0.49
1:B:106:ASP:HB3	1:B:109:SER:HB3	1.95	0.49
1:A:401:PHE:CE1	1:A:429:VAL:HG21	2.45	0.49
2:D:6:C:C6	2:D:6:C:H5'	2.36	0.49
1:B:741:ARG:O	1:B:745:GLU:HG2	2.12	0.49
1:A:106:ASP:HB3	1:A:109:SER:CB	2.36	0.49
1:B:558:PHE:CD1	1:B:559:PRO:CD	2.95	0.49
1:A:744:VAL:CG2	1:A:745:GLU:N	2.76	0.48
1:A:632:ILE:HD11	2:D:14:A:N1	2.28	0.48
1:B:209:LEU:HG	1:B:213:ASN:HD21	1.77	0.48
1:A:142:GLU:CG	1:A:172:LEU:HD23	2.41	0.48
1:A:743:VAL:HG23	1:A:744:VAL:N	2.28	0.48
1:A:635:ASN:OD1	1:A:669:SER:OG	2.14	0.48
1:A:718:PHE:CG	1:A:747:TYR:CZ	3.01	0.48
1:B:375:GLN:O	1:B:379:THR:HG23	2.13	0.48
1:B:745:GLU:O	1:B:749:ARG:HG3	2.14	0.48
1:B:330:PHE:CD2	1:B:333:GLU:HB2	2.48	0.48
1:B:413:ARG:HG3	1:B:413:ARG:O	2.13	0.48
1:A:641:TYR:HB3	1:A:646:GLU:O	2.13	0.48
1:B:525:GLU:OE1	1:B:560:SER:CB	2.61	0.48
1:A:657:LEU:O	1:A:665:PRO:HD3	2.14	0.48
1:B:223:GLY:O	1:B:225:SER:OG	2.24	0.48
1:B:243:PRO:HB3	1:B:247:THR:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:SER:OG	1:B:430:SER:O	2.32	0.48
1:A:98:ARG:NH2	1:A:101:GLU:OE2	2.47	0.48
1:B:565:ARG:O	1:B:569:ILE:HG13	2.14	0.48
2:D:12:U:H4'	2:D:14:A:C5'	2.44	0.48
1:A:690:LEU:O	1:A:694:VAL:HG23	2.14	0.48
1:A:106:ASP:O	1:A:109:SER:HB2	2.14	0.47
1:B:213:ASN:O	4:B:901:HOH:O	2.20	0.47
1:A:79:LEU:HD12	1:A:98:ARG:CZ	2.30	0.47
1:B:287:LEU:CD1	1:B:317:THR:OG1	2.62	0.47
1:A:632:ILE:HD13	2:D:14:A:N3	2.29	0.47
1:A:677:PHE:O	1:A:681:GLY:N	2.46	0.47
1:B:161:LEU:HD13	1:B:180:VAL:HG11	1.95	0.47
1:B:623:LYS:O	1:B:626:GLY:N	2.30	0.47
1:A:341:MET:HE3	1:A:348:PRO:HG3	1.95	0.47
1:A:736:MET:HG3	1:A:739:THR:OG1	2.14	0.47
1:B:161:LEU:CD1	1:B:180:VAL:HG11	2.44	0.47
1:A:119:HIS:CD2	1:A:122:TRP:CE3	3.03	0.47
1:A:510:GLN:O	1:A:513:VAL:HG12	2.14	0.47
1:A:106:ASP:CG	1:A:109:SER:HB2	2.34	0.47
1:B:513:VAL:HA	1:B:516:MET:SD	2.55	0.47
1:A:609:ASN:N	1:A:609:ASN:OD1	2.47	0.47
1:B:604:SER:OG	1:B:636:SER:HB3	2.15	0.47
1:B:490:ILE:HG22	1:B:494:ASN:HD21	1.80	0.47
1:B:352:THR:O	1:B:356:VAL:HG23	2.14	0.47
1:B:360:TYR:HB3	1:B:365:LYS:O	2.15	0.47
1:A:497:LEU:HB2	1:A:530:LEU:HD23	1.97	0.47
1:A:738:LEU:HD23	1:A:738:LEU:O	2.15	0.47
1:A:740:TYR:CA	1:A:743:VAL:HG22	2.45	0.47
1:B:314:ASP:C	1:B:317:THR:HG23	2.35	0.47
1:A:374:ASP:O	1:A:378:LYS:HD2	2.15	0.47
1:A:116:LEU:HG	1:A:116:LEU:O	2.13	0.47
1:A:307:GLU:O	1:A:310:GLY:N	2.48	0.47
1:A:513:VAL:HG23	1:A:516:MET:HE3	1.97	0.47
1:A:124:LEU:O	1:A:128:ARG:HG3	2.14	0.47
1:B:453:LEU:HD12	1:B:453:LEU:H	1.80	0.47
1:B:775:LEU:O	1:B:778:TYR:N	2.48	0.47
1:A:141:LEU:CD2	1:A:166:LEU:HD11	2.45	0.46
1:A:706:HIS:HE1	1:A:738:LEU:CG	2.18	0.46
1:B:283:TYR:O	1:B:287:LEU:HB2	2.16	0.46
1:B:107:ILE:HD12	1:B:107:ILE:H	1.78	0.46
1:A:313:PRO:HB3	1:A:317:THR:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:VAL:HG22	1:A:563:ILE:HD13	1.90	0.46
1:B:575:ARG:HD3	1:B:605:ILE:HD13	1.97	0.46
1:A:515:LYS:NZ	1:A:519:LYS:HD3	2.31	0.46
1:B:599:PHE:CB	1:B:622:ILE:CD1	2.81	0.46
1:A:560:SER:O	1:A:561:TRP:C	2.53	0.46
1:B:376:MET:CE	1:B:381:PHE:CZ	2.98	0.46
1:B:298:GLU:C	1:B:300:LEU:N	2.69	0.46
1:A:314:ASP:OD1	1:A:317:THR:OG1	2.34	0.46
1:A:98:ARG:O	1:A:102:LEU:HG	2.15	0.46
1:B:283:TYR:CD1	1:B:306:MET:HA	2.51	0.46
1:B:659:CYS:O	1:B:661:GLN:N	2.48	0.46
1:A:129:TRP:CZ2	1:A:133:GLU:OE1	2.69	0.46
1:B:368:GLU:OE1	1:B:368:GLU:N	2.49	0.46
1:A:548:GLU:HB3	1:A:552:TYR:CE2	2.51	0.46
2:D:14:A:C8	2:D:14:A:H3'	2.51	0.46
1:A:200:LEU:O	1:A:205:VAL:HB	2.15	0.46
2:D:6:C:C5'	2:D:6:C:C6	2.86	0.46
1:B:606:TYR:O	1:B:611:MET:O	2.33	0.46
1:A:142:GLU:HG3	1:A:172:LEU:CD2	2.46	0.46
1:A:653:ILE:HA	1:A:656:GLN:HB2	1.98	0.46
1:A:760:LEU:HD12	1:A:761:SER:N	2.30	0.45
1:B:590:ARG:NH1	4:B:933:HOH:O	2.45	0.45
1:A:419:ASN:HD22	1:A:422:THR:H	1.60	0.45
1:A:451:VAL:HG13	1:A:451:VAL:O	2.17	0.45
1:B:306:MET:CE	1:B:317:THR:HG21	2.46	0.45
1:B:562:VAL:HG23	1:B:563:ILE:H	1.81	0.45
1:A:141:LEU:HD23	1:A:172:LEU:HD21	1.98	0.45
2:D:16:U:H5'	4:D:102:HOH:O	2.16	0.45
1:A:668:VAL:HG13	2:D:16:U:N1	2.31	0.45
1:B:455:ARG:NE	1:B:489:CYS:SG	2.90	0.45
1:A:636:SER:CB	4:A:811:HOH:O	2.64	0.45
1:A:212:TYR:CD1	1:A:236:MET:HB3	2.52	0.45
1:B:127:LEU:HD11	1:B:141:LEU:HA	1.97	0.45
1:A:296:TYR:CE1	1:A:300:LEU:HD21	2.51	0.45
2:D:10:A:H8	2:D:10:A:OP2	2.00	0.45
1:A:338:LEU:CD2	1:A:375:GLN:HB3	2.46	0.45
1:B:262:ASP:CB	4:B:919:HOH:O	2.63	0.45
1:B:277:ALA:HA	1:B:278:PRO:HD2	1.81	0.45
1:A:594:PRO:HG2	1:A:599:PHE:CZ	2.51	0.45
1:B:743:VAL:O	1:B:747:TYR:HB2	2.17	0.45
1:A:709:VAL:HG13	1:A:721:ALA:HB1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:GLU:H	1:B:121:GLU:HG2	1.54	0.45
1:B:219:TYR:HA	1:B:222:MET:HE2	1.98	0.45
1:A:370:LEU:HD12	1:A:370:LEU:HA	1.83	0.45
2:D:14:A:H8	2:D:14:A:H3'	1.82	0.45
1:B:666:ASP:C	1:B:668:VAL:N	2.69	0.45
1:A:237:ARG:CZ	1:A:274:ARG:NH1	2.80	0.45
2:D:13:U:H3'	2:D:13:U:C6	2.52	0.45
1:A:348:PRO:O	1:A:381:PHE:CE2	2.70	0.45
1:B:441:ARG:HA	1:B:441:ARG:HD3	1.74	0.45
1:B:161:LEU:HD13	1:B:180:VAL:CG1	2.46	0.45
1:A:692:GLU:HA	1:A:695:ALA:HB3	1.99	0.45
1:A:715:LEU:HB3	1:A:717:MET:CG	2.47	0.45
1:B:654:LEU:CD2	1:B:658:LYS:HE3	2.46	0.45
1:A:454:SER:H	1:A:457:THR:HG1	1.61	0.45
1:A:287:LEU:HD13	1:A:299:ALA:CB	2.40	0.44
1:A:612:TYR:HA	1:A:640:MET:HE1	2.00	0.44
1:A:387:THR:O	1:A:391:VAL:HG23	2.17	0.44
1:B:197:PHE:O	1:B:200:LEU:HB3	2.16	0.44
1:A:104:ARG:HB2	4:A:807:HOH:O	2.16	0.44
1:B:284:ASN:N	1:B:284:ASN:ND2	2.63	0.44
1:B:577:LEU:CD2	1:B:611:MET:CE	2.93	0.44
2:D:13:U:C6	2:D:13:U:C3'	2.99	0.44
1:A:777:ALA:O	1:A:781:ASP:N	2.49	0.44
1:B:637:LEU:HA	1:B:637:LEU:HD23	1.72	0.44
1:A:268:PHE:CD2	1:A:286:LEU:HD22	2.52	0.44
1:A:161:LEU:HD22	1:A:184:LEU:HD21	1.98	0.44
1:A:101:GLU:HA	4:A:807:HOH:O	2.16	0.44
1:B:559:PRO:HB2	1:B:564:LEU:HD21	1.98	0.44
1:A:548:GLU:HB3	1:A:552:TYR:HE2	1.82	0.44
1:A:610:GLY:O	1:A:612:TYR:N	2.48	0.44
1:A:578:ASP:N	1:A:578:ASP:OD1	2.49	0.44
1:B:501:SER:HA	1:B:534:CYS:SG	2.57	0.44
1:A:86:HIS:CG	1:A:87:PRO:HD2	2.52	0.44
1:A:338:LEU:CD2	1:A:375:GLN:HG2	2.46	0.44
1:B:614:LYS:O	1:B:617:GLU:HB2	2.17	0.44
1:A:720:GLU:HG2	1:A:720:GLU:H	1.58	0.44
1:A:706:HIS:O	1:A:706:HIS:CD2	2.70	0.44
1:A:296:TYR:O	1:A:296:TYR:CD1	2.70	0.44
1:B:577:LEU:HD22	1:B:609:ASN:ND2	2.33	0.44
1:B:283:TYR:HB3	1:B:306:MET:CG	2.34	0.44
1:B:660:SER:O	1:B:662:THR:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:PHE:HZ	1:B:371:ALA:CB	2.25	0.44
1:B:211:THR:O	1:B:215:VAL:HG23	2.18	0.44
1:B:400:ARG:O	1:B:404:MET:HG3	2.18	0.44
1:A:221:ARG:HD3	4:A:835:HOH:O	2.17	0.43
1:A:338:LEU:HD22	1:A:375:GLN:CG	2.48	0.43
1:A:288:GLN:HG3	2:C:5:U:C5'	2.48	0.43
2:D:6:C:C6	2:D:6:C:C4'	3.02	0.43
1:A:291:GLY:CA	1:A:324:THR:CG2	2.87	0.43
1:A:348:PRO:O	1:A:381:PHE:CZ	2.72	0.43
1:A:754:GLU:C	1:A:756:ALA:N	2.71	0.43
1:A:431:GLY:O	1:A:432:LYS:HB2	2.19	0.43
1:A:288:GLN:HG3	2:C:5:U:H5'	1.99	0.43
1:B:167:PRO:O	1:B:170:SER:OG	2.17	0.43
1:A:270:ASP:O	1:A:274:ARG:CG	2.66	0.43
1:B:519:LYS:HB3	1:B:521:PHE:CD2	2.53	0.43
1:B:478:TYR:O	1:B:482:THR:HG23	2.18	0.43
1:B:490:ILE:HG22	1:B:494:ASN:ND2	2.33	0.43
1:B:172:LEU:HB2	1:B:177:TYR:CE2	2.54	0.43
1:A:291:GLY:HA3	1:A:324:THR:HG23	1.93	0.43
1:B:543:GLY:O	1:B:547:ILE:HG13	2.18	0.43
1:A:655:ASN:HA	1:A:658:LYS:HE3	2.01	0.43
1:A:706:HIS:CE1	1:A:738:LEU:HB3	2.53	0.43
1:A:175:ARG:O	1:A:179:THR:OG1	2.35	0.43
1:B:532:LEU:HD12	1:B:547:ILE:HD12	2.00	0.43
1:A:571:ASN:O	1:A:576:ARG:N	2.37	0.43
1:B:660:SER:OG	1:B:663:MET:N	2.45	0.43
1:B:114:LEU:HD22	1:B:122:TRP:CB	2.49	0.43
1:A:377:LYS:C	1:A:379:THR:N	2.72	0.43
1:A:634:TYR:HB3	1:A:657:LEU:HD11	2.01	0.42
1:B:537:LYS:HB3	1:B:537:LYS:HE3	1.81	0.42
1:A:619:PHE:O	1:A:622:ILE:HB	2.19	0.42
1:A:687:GLN:HE21	1:A:708:LEU:HD11	1.83	0.42
1:A:684:LYS:HG3	1:A:685:GLU:N	2.32	0.42
1:B:659:CYS:C	1:B:661:GLN:N	2.71	0.42
1:B:676:GLY:O	1:B:680:GLN:HG3	2.19	0.42
1:B:757:ARG:NH1	1:B:780:GLU:OE1	2.52	0.42
1:B:654:LEU:O	1:B:657:LEU:HB2	2.19	0.42
2:D:14:A:HO2'	2:D:15:U:P	2.38	0.42
1:B:116:LEU:HD23	1:B:116:LEU:HA	1.77	0.42
1:A:243:PRO:HB3	1:A:247:THR:HG21	2.01	0.42
1:A:79:LEU:HA	1:A:79:LEU:HD12	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:MET:HE2	1:A:348:PRO:HG3	1.99	0.42
1:B:575:ARG:NH1	1:B:608:LYS:HE3	2.34	0.42
1:A:340:THR:C	1:A:342:ALA:N	2.73	0.42
1:B:752:ARG:H	1:B:752:ARG:HG2	1.57	0.42
1:A:95:LEU:HD22	1:A:126:LEU:HD13	2.01	0.42
1:A:300:LEU:HD23	1:A:321:LEU:CD2	2.49	0.42
1:B:178:THR:CG2	1:B:211:THR:OG1	2.67	0.42
1:A:761:SER:C	1:A:763:VAL:H	2.22	0.42
2:D:5:U:C2'	2:D:6:C:C5'	2.86	0.42
1:A:338:LEU:HD21	1:A:375:GLN:CB	2.48	0.42
1:A:253:ALA:O	1:A:257:ARG:HG3	2.19	0.42
1:B:415:GLY:O	1:B:417:THR:N	2.52	0.42
1:A:524:ASN:ND2	1:A:524:ASN:N	2.68	0.42
1:B:667:VAL:HA	1:B:670:TYR:HD2	1.85	0.42
1:B:559:PRO:CD	1:B:590:ARG:HH22	2.30	0.42
1:B:559:PRO:CD	1:B:590:ARG:NH2	2.83	0.42
1:B:575:ARG:HD3	1:B:575:ARG:HA	1.66	0.42
1:B:298:GLU:O	1:B:300:LEU:N	2.52	0.42
1:B:660:SER:C	1:B:662:THR:N	2.70	0.42
1:A:288:GLN:OE1	1:A:292:LYS:HE2	2.20	0.42
1:A:663:MET:HB2	1:A:663:MET:HE2	1.99	0.42
1:A:500:LEU:HD22	1:A:505:ASP:HB3	2.02	0.42
1:A:725:ILE:C	1:A:727:TYR:N	2.73	0.41
1:B:260:LEU:HB3	1:B:263:GLU:CG	2.48	0.41
1:A:733:LEU:HA	1:A:733:LEU:HD23	1.88	0.41
1:B:314:ASP:O	1:B:317:THR:HG23	2.20	0.41
1:B:535:TYR:CZ	1:B:543:GLY:HA3	2.55	0.41
1:A:353:TYR:CD1	1:A:372:LEU:HD21	2.55	0.41
1:B:353:TYR:HB3	1:B:376:MET:HE3	2.02	0.41
1:A:660:SER:C	1:A:662:THR:N	2.73	0.41
1:B:715:LEU:HD12	1:B:717:MET:CE	2.49	0.41
1:B:581:GLU:O	1:B:582:THR:C	2.57	0.41
1:A:98:ARG:NH2	1:A:101:GLU:CD	2.72	0.41
1:B:175:ARG:NH2	2:D:1:G:O5'	2.45	0.41
1:A:545:ALA:HA	1:A:548:GLU:HG3	2.02	0.41
2:D:14:A:O2'	2:D:15:U:P	2.78	0.41
1:B:176:ALA:O	1:B:180:VAL:HG23	2.20	0.41
1:B:248:ALA:O	1:B:252:ILE:HG13	2.20	0.41
1:A:74:PRO:C	1:A:76:ALA:H	2.24	0.41
1:A:524:ASN:ND2	1:B:590:ARG:O	2.54	0.41
1:B:753:PHE:CD2	1:B:783:GLN:CG	2.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:TYR:CD2	1:A:376:MET:HG3	2.56	0.41
1:B:690:LEU:O	1:B:693:MET:HB3	2.20	0.41
1:A:173:ASP:O	1:A:177:TYR:HD2	2.02	0.41
1:A:74:PRO:HG2	1:A:75:ASP:H	1.85	0.41
1:A:316:VAL:O	1:A:320:GLU:HG3	2.21	0.41
1:A:660:SER:O	1:A:662:THR:N	2.54	0.41
1:B:753:PHE:CE2	1:B:783:GLN:CA	2.87	0.41
1:B:281:VAL:HG11	2:D:3:A:C2	2.55	0.41
1:A:692:GLU:O	1:A:695:ALA:N	2.53	0.41
1:B:564:LEU:HB3	1:B:587:VAL:HG22	2.03	0.41
2:D:9:U:O4'	2:D:9:U:P	2.78	0.41
1:B:284:ASN:ND2	1:B:317:THR:HB	2.36	0.41
1:A:585:GLN:NE2	1:A:586:GLU:OE2	2.53	0.41
1:B:715:LEU:O	1:B:716:GLU:O	2.39	0.41
1:B:747:TYR:HB3	1:B:756:ALA:HB2	2.03	0.41
1:B:96:ALA:O	1:B:99:ARG:HB2	2.21	0.41
1:A:435:MET:O	1:A:439:VAL:HG23	2.20	0.41
1:A:341:MET:O	1:A:341:MET:SD	2.79	0.41
1:B:661:GLN:HE21	1:B:661:GLN:HB3	1.53	0.41
1:A:560:SER:O	1:A:563:ILE:N	2.52	0.41
1:A:400:ARG:O	1:A:404:MET:HG3	2.21	0.41
1:A:660:SER:OG	1:A:663:MET:N	2.45	0.41
1:A:761:SER:C	1:A:763:VAL:N	2.74	0.41
1:B:623:LYS:C	1:B:625:SER:N	2.73	0.41
1:B:635:ASN:HA	1:B:635:ASN:HD22	1.58	0.41
1:B:478:TYR:CD1	1:B:496:LEU:HD11	2.56	0.41
1:B:482:THR:OG1	1:B:483:SER:N	2.53	0.41
1:B:655:ASN:HA	1:B:655:ASN:HD22	1.60	0.41
1:A:267:PHE:O	1:A:271:LEU:HB2	2.21	0.41
1:A:737:GLU:N	1:A:737:GLU:OE1	2.54	0.41
1:A:598:ILE:O	1:A:602:MET:HG2	2.20	0.41
1:B:246:PHE:CE2	2:D:3:A:C5	3.09	0.41
1:B:605:ILE:HD12	1:B:605:ILE:HA	1.80	0.41
1:B:398:LYS:HD3	1:B:398:LYS:HA	1.58	0.41
1:A:338:LEU:CD2	1:A:375:GLN:HB2	2.50	0.40
1:A:174:VAL:HG21	1:A:208:THR:CG2	2.50	0.40
1:B:664:LYS:C	1:B:665:PRO:O	2.59	0.40
1:B:281:VAL:HG23	2:D:4:U:C2	2.56	0.40
1:A:775:LEU:C	1:A:777:ALA:H	2.24	0.40
1:B:154:HIS:CD2	1:B:186:ARG:HG2	2.57	0.40
1:A:127:LEU:HD23	1:A:127:LEU:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:VAL:HA	1:B:406:GLU:HB2	2.03	0.40
1:A:287:LEU:HD13	1:A:299:ALA:CA	2.51	0.40
1:B:560:SER:OG	1:B:562:VAL:CG2	2.69	0.40
1:A:657:LEU:O	1:A:663:MET:O	2.39	0.40
1:A:260:LEU:HB3	1:A:263:GLU:HG2	2.02	0.40
1:B:191:GLU:O	1:B:195:GLU:HG3	2.20	0.40
1:B:743:VAL:O	1:B:747:TYR:N	2.52	0.40
1:A:728:MET:O	1:A:732:GLY:N	2.54	0.40
1:B:541:VAL:HG13	1:B:576:ARG:NE	2.37	0.40
1:B:495:ALA:O	1:B:498:ASN:HB3	2.21	0.40
1:B:73:SER:HA	1:B:74:PRO:HD3	1.90	0.40
1:A:394:MET:HB3	1:A:394:MET:HE3	1.96	0.40
1:A:608:LYS:CG	4:A:841:HOH:O	2.67	0.40
1:A:271:LEU:HD12	1:A:271:LEU:HA	1.85	0.40
1:B:733:LEU:HA	1:B:733:LEU:HD13	1.72	0.40
1:B:319:ASN:O	1:B:322:ALA:HB3	2.20	0.40

All (1) 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:168:PRO:O	1:A:447:ARG:NH1[1_455]	1.93	0.27

## 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	
1	A	677/718 (94%)	599 (88%)	65 (10%)	13 (2%)	10	8
1	B	671/718 (94%)	605 (90%)	50 (8%)	16 (2%)	7	4
All	All	1348/1436 (94%)	1204 (89%)	115 (8%)	29 (2%)	8	6

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	168	PRO
1	B	315	ALA
1	B	665	PRO
1	A	511	SER
1	A	698	MET
1	A	739	THR
1	B	169	GLY
1	B	300	LEU
1	B	380	GLY
1	B	416	CYS
1	B	716	GLU
1	A	341	MET
1	A	505	ASP
1	B	314	ASP
1	A	378	LYS
1	A	554	SER
1	A	734	LYS
1	A	749	ARG
1	B	299	ALA
1	B	663	MET
1	B	664	LYS
1	A	164	THR
1	B	170	SER
1	B	224	ARG
1	B	451	VAL
1	A	726	GLY
1	A	735	PRO
1	A	553	GLY
1	B	734	LYS

### 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
1	A	539/587 (92%)	455 (84%)	84 (16%)	<b>3</b> <b>2</b>

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	530/587 (90%)	476 (90%)	54 (10%)	9 10
All	All	1069/1174 (91%)	931 (87%)	138 (13%)	5 4

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	LEU
1	A	97	SER
1	A	99	ARG
1	A	109	SER
1	A	124	LEU
1	A	127	LEU
1	A	133	GLU
1	A	139	SER
1	A	143	MET
1	A	146	ARG
1	A	163	GLU
1	A	164	THR
1	A	173	ASP
1	A	174	VAL
1	A	175	ARG
1	A	178	THR
1	A	192	ARG
1	A	200	LEU
1	A	208	THR
1	A	242	GLU
1	A	263	GLU
1	A	279	SER
1	A	280	VAL
1	A	287	LEU
1	A	298	GLU
1	A	303	LEU
1	A	311	CYS
1	A	338	LEU
1	A	340	THR
1	A	341	MET
1	A	349	ASN
1	A	356	VAL
1	A	358	THR
1	A	367	ASP
1	A	370	LEU
1	A	378	LYS

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Mol	Chain	Res	Type
1	A	398	LYS
1	A	419	ASN
1	A	420	ARG
1	A	426	MET
1	A	430	SER
1	A	433	ARG
1	A	457	THR
1	A	460	THR
1	A	465	TYR
1	A	477	MET
1	A	489	CYS
1	A	491	THR
1	A	519	LYS
1	A	527	SER
1	A	529	SER
1	A	534	CYS
1	A	560	SER
1	A	577	LEU
1	A	593	ASN
1	A	595	ASP
1	A	601	SER
1	A	609	ASN
1	A	624	ARG
1	A	628	SER
1	A	637	LEU
1	A	640	MET
1	A	643	LYS
1	A	652	LYS
1	A	659	CYS
1	A	662	THR
1	A	663	MET
1	A	715	LEU
1	A	717	MET
1	A	719	SER
1	A	720	GLU
1	A	727	TYR
1	A	728	MET
1	A	729	VAL
1	A	737	GLU
1	A	739	THR
1	A	742	ARG
1	A	747	TYR

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Mol	Chain	Res	Type
1	A	748	CYS
1	A	749	ARG
1	A	761	SER
1	A	762	GLU
1	A	775	LEU
1	A	778	TYR
1	B	72	LEU
1	B	73	SER
1	B	88	LEU
1	B	114	LEU
1	B	115	GLU
1	B	121	GLU
1	B	127	LEU
1	B	146	ARG
1	B	164	THR
1	B	175	ARG
1	B	178	THR
1	B	186	ARG
1	B	191	GLU
1	B	201	ARG
1	B	281	VAL
1	B	284	ASN
1	B	286	LEU
1	B	287	LEU
1	B	292	LYS
1	B	306	MET
1	B	327	ARG
1	B	330	PHE
1	B	341	MET
1	B	363	VAL
1	B	367	ASP
1	B	372	LEU
1	B	378	LYS
1	B	385	VAL
1	B	390	LEU
1	B	398	LYS
1	B	413	ARG
1	B	416	CYS
1	B	424	ASN
1	B	429	VAL
1	B	455	ARG
1	B	491	THR

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Mol	Chain	Res	Type
1	B	503	GLN
1	B	550	GLU
1	B	562	VAL
1	B	575	ARG
1	B	585	GLN
1	B	608	LYS
1	B	624	ARG
1	B	625	SER
1	B	631	LEU
1	B	637	LEU
1	B	656	GLN
1	B	715	LEU
1	B	716	GLU
1	B	733	LEU
1	B	747	TYR
1	B	752	ARG
1	B	757	ARG
1	B	780	GLU

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

Mol	Chain	Res	Type
1	A	77	GLN
1	A	203	GLN
1	A	309	ASN
1	A	419	ASN
1	A	524	ASN
1	A	675	ASN
1	A	687	GLN
1	A	706	HIS
1	A	731	HIS
1	B	77	GLN
1	B	153	GLN
1	B	154	HIS
1	B	284	ASN
1	B	503	GLN
1	B	635	ASN
1	B	655	ASN
1	B	656	GLN
1	B	661	GLN
1	B	706	HIS



### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	12/18 (66%)	5 (41%)	2 (16%)
2	D	17/18 (94%)	9 (52%)	3 (17%)
All	All	29/36 (80%)	14 (48%)	5 (17%)

All (14) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	D	6	C
2	D	7	U
2	D	9	U
2	D	10	A
2	D	11	A
2	D	13	U
2	D	14	A
2	D	15	U
2	D	18	C
2	C	5	U
2	C	12	U
2	C	13	U
2	C	14	A
2	C	15	U

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	D	5	U
2	D	9	U
2	D	14	A
2	C	12	U
2	C	13	U

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

1 ligand is modelled in this entry.

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	$\# Z  > 2$
3	PO4	B	801	-	4,4,4	0.48	0	6,6,6	0.27	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	B	801	-	-	0/0/0/0	0/0/0/0

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	A	687/718 (95%)	0.42	56 (8%) 14 15	47, 84, 146, 362	103 (14%)
1	B	683/718 (95%)	0.34	53 (7%) 16 16	41, 84, 133, 274	86 (12%)
2	C	14/18 (77%)	-0.03	1 (7%) 19 20	61, 87, 111, 130	4 (28%)
2	D	18/18 (100%)	0.67	3 (16%) 2 2	73, 93, 148, 159	6 (33%)
All	All	1402/1472 (95%)	0.38	113 (8%) 15 15	41, 84, 140, 362	199 (14%)

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	329	GLY	14.7
1	A	712	TYR	9.6
1	B	784	PHE	8.3
1	A	296	TYR	6.5
1	A	324	THR	6.5
1	B	331	PHE	6.5
1	B	747	TYR	5.6
1	A	713	SER	5.5
2	D	13	U	5.5
1	A	172	LEU	5.3
1	A	740	TYR	5.1
1	A	778	TYR	4.9
1	A	750	ALA	4.9
1	B	281	VAL	4.9
1	B	327	ARG	4.7
1	A	748	CYS	4.7
1	A	116	LEU	4.7
1	A	341	MET	4.6
1	A	759	PHE	4.6
1	A	719	SER	4.6
1	B	328	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	334	ALA	4.5
1	B	744	VAL	4.4
1	A	273	ALA	4.4
1	A	682	LEU	4.3
1	B	268	PHE	4.3
1	A	775	LEU	4.3
1	B	775	LEU	4.2
1	A	652	LYS	4.2
1	B	716	GLU	4.1
1	B	780	GLU	4.1
1	B	306	MET	4.0
1	A	747	TYR	3.9
1	B	351	PHE	3.8
1	A	381	PHE	3.8
1	B	750	ALA	3.7
1	A	718	PHE	3.7
1	B	622	ILE	3.7
1	A	372	LEU	3.7
1	B	587	VAL	3.7
1	B	715	LEU	3.7
1	B	749	ARG	3.6
1	A	761	SER	3.5
1	B	287	LEU	3.4
1	A	269	GLU	3.4
1	B	293	ALA	3.4
1	A	163	GLU	3.3
1	B	782	ALA	3.2
1	B	673	VAL	3.2
1	B	627	LEU	3.2
1	B	265	VAL	3.2
1	A	724	VAL	3.1
1	B	611	MET	3.0
1	B	381	PHE	3.0
1	B	689	VAL	3.0
1	B	714	SER	3.0
1	A	278	PRO	3.0
1	B	746	SER	2.9
1	B	759	PHE	2.9
1	A	338	LEU	2.9
1	B	682	LEU	2.8
1	A	292	LYS	2.8
1	A	224	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	708	LEU	2.8
1	A	351	PHE	2.8
1	A	293	ALA	2.8
1	A	756	ALA	2.8
1	B	760	LEU	2.7
1	A	716	GLU	2.7
1	B	357	MET	2.7
1	A	363	VAL	2.7
1	A	593	ASN	2.6
1	B	708	LEU	2.6
1	A	703	VAL	2.6
1	B	557	VAL	2.6
1	A	428	ALA	2.6
1	A	379	THR	2.5
1	B	748	CYS	2.5
1	A	684	LYS	2.5
1	B	648	TRP	2.5
1	A	115	GLU	2.4
1	B	752	ARG	2.4
1	B	277	ALA	2.4
1	A	294	GLY	2.4
2	D	10	A	2.4
1	A	177	TYR	2.3
1	B	606	TYR	2.3
1	B	299	ALA	2.3
2	D	8	U	2.3
1	A	728	MET	2.3
1	B	353	TYR	2.3
1	A	744	VAL	2.3
1	A	558	PHE	2.3
1	A	287	LEU	2.3
1	A	657	LEU	2.3
1	B	322	ALA	2.2
1	A	686	ALA	2.2
1	B	168	PRO	2.2
1	B	330	PHE	2.2
2	C	13	U	2.2
1	B	431	GLY	2.2
1	A	663	MET	2.2
1	B	558	PHE	2.1
1	B	591	GLY	2.1
1	A	286	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	776	GLU	2.1
1	B	115	GLU	2.1
1	B	743	VAL	2.1
1	B	751	LYS	2.1
1	A	173	ASP	2.1
1	A	478	TYR	2.0
1	A	527	SER	2.0
1	A	364	GLY	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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	PO4	B	801	5/5	0.93	0.13	-1.68	82,82,82,82	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.