



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 05:21 am BST

PDB ID : 4OE1
Title : Crystal structure of the pentatricopeptide repeat protein PPR10 (C256S/C430S/C449S) in complex with an 18-nt PSAJ rna element
Authors : Li, Q.; Yan, C.; Wu, J.; Yin, P.; Yan, N.
Deposited on : 2014-01-11
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

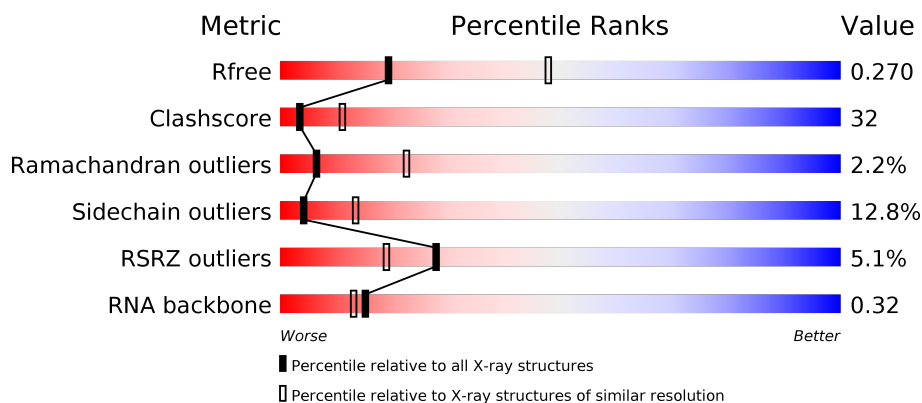
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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 ≥ 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	718	<div> <div>5%</div> <div>49%</div> <div>38%</div> <div>7%</div> <div>• •</div> </div>
1	B	718	<div> <div>5%</div> <div>56%</div> <div>33%</div> <div>6%</div> <div>5%</div> </div>
2	C	18	<div> <div>44%</div> <div>11%</div> <div>22%</div> <div>22%</div> </div>
2	D	18	<div> <div>6%</div> <div>11%</div> <div>39%</div> <div>50%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11033 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	16	0	0
			5202	3284	890	985	43			
1	B	683	Total	C	N	O	S	14	0	0
			5179	3273	891	973	42			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	256	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	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	3	0	0
			368	167	53	131	17			
2	C	14	Total	C	N	O	P	4	0	0
			279	126	41	99	13			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

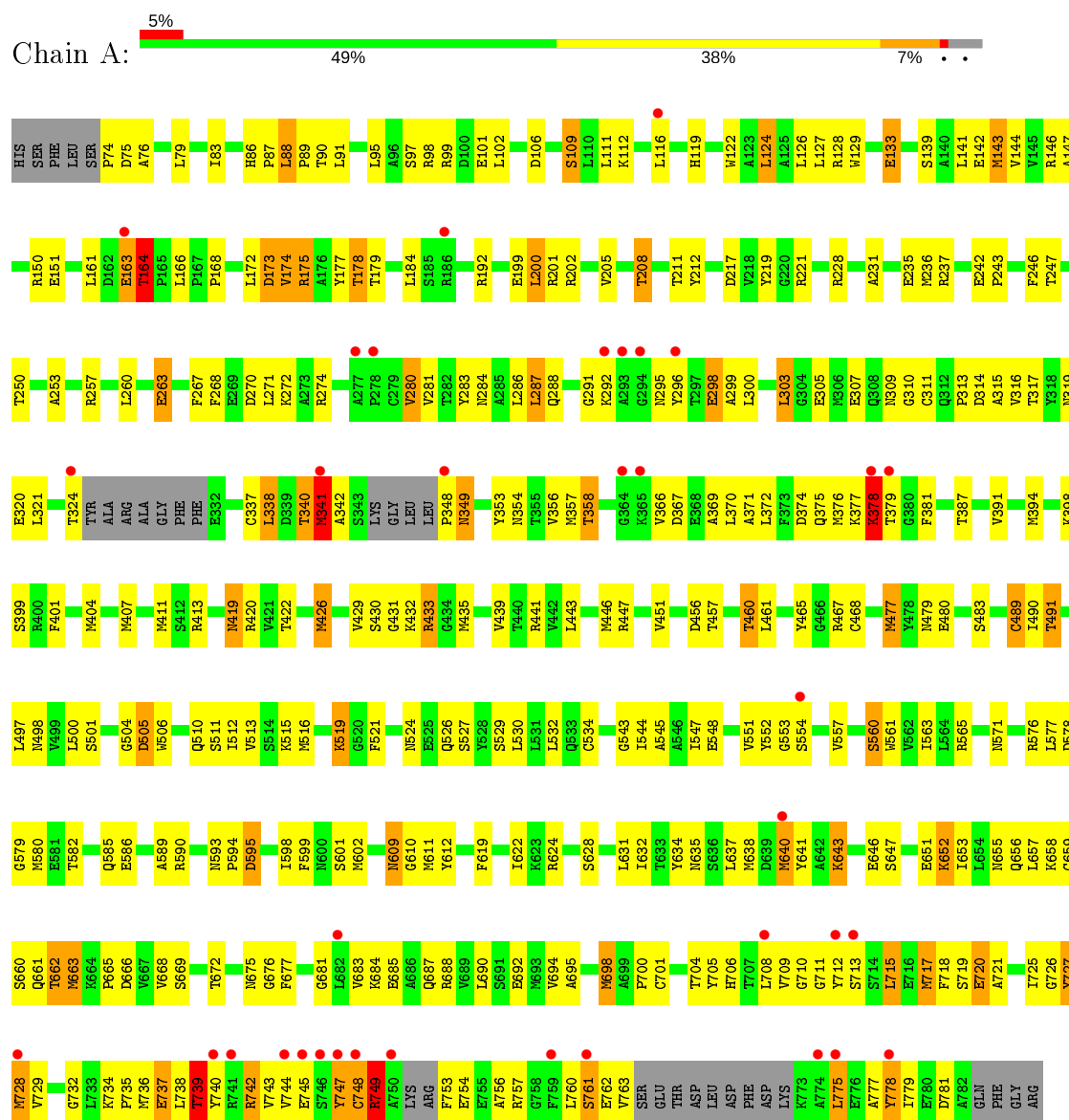


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	5	0
			5	4	1		

3 Residue-property plots [i](#)

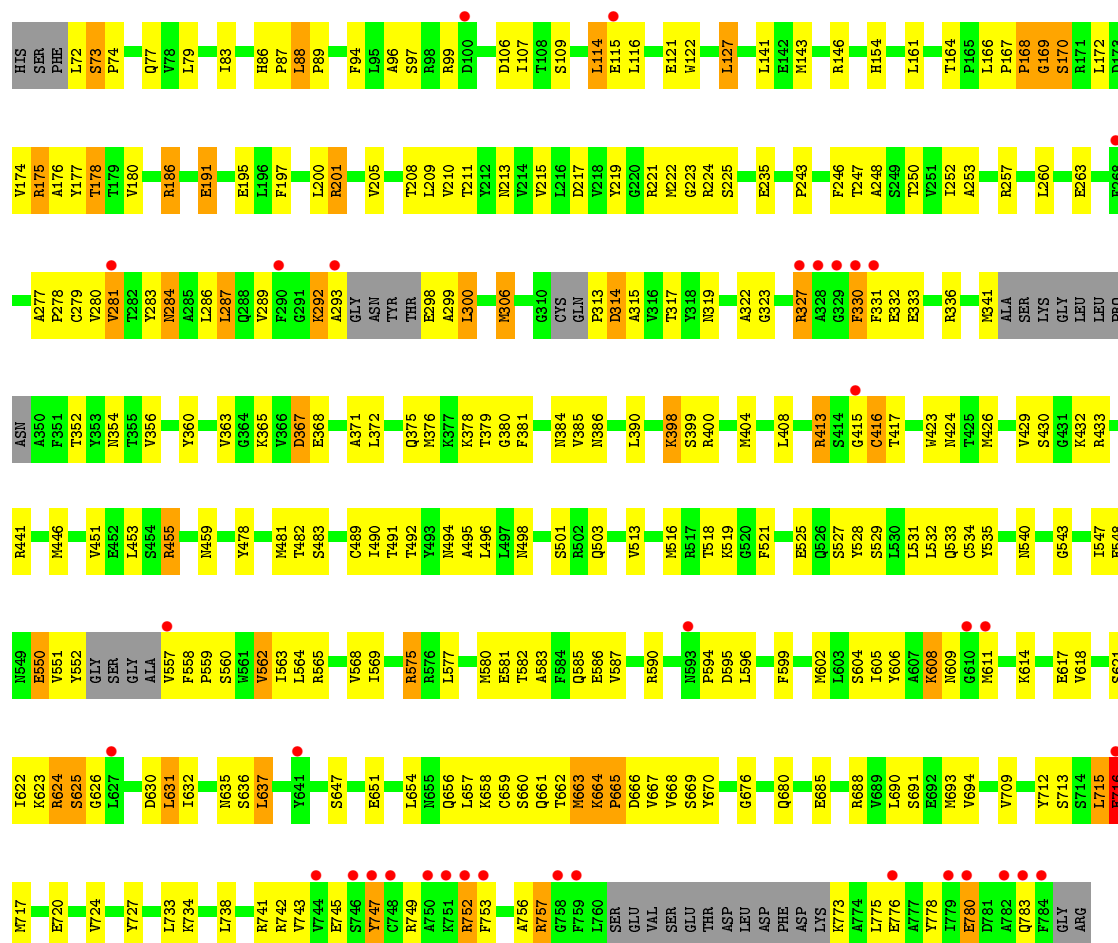
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Chloroplast pentatricopeptide repeat protein 10

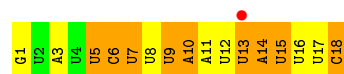


- Molecule 1: Chloroplast pentatricopeptide repeat protein 10

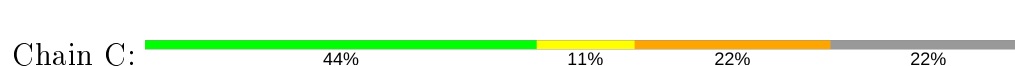




• Molecule 2: psaJ RNA



• Molecule 2: psaJ RNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	83.32Å 83.32Å 225.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.26 – 2.80 34.26 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (34.26-2.80) 98.2 (34.26-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.263 , 0.278 0.257 , 0.270	Depositor DCC
R_{free} test set	1855 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	67.0	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.054 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11033	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.72	1/5294 (0.0%)	0.53	0/7177
1	B	0.78	1/5269 (0.0%)	0.58	1/7136 (0.0%)
2	C	0.27	0/308	0.72	0/474
2	D	0.33	0/408	0.66	0/631
All	All	0.73	2/11279 (0.0%)	0.56	1/15418 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	548	GLU	C-N	-7.04	1.17	1.34
1	A	468	CYS	CB-SG	-5.76	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	6.03	110.54	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	380	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5179	0	5067	272	1
2	C	279	0	146	10	0
2	D	368	0	189	60	0
3	B	5	0	0	0	0
All	All	11033	0	10508	688	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 32.

All (688) 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	1.59
1:A:489:CYS:SG	1:A:491:THR:HG22	1.50	1.51
1:A:79:LEU:HD13	1:A:98:ARG:NH2	1.32	1.43
1:A:515:LYS:NZ	1:A:519:LYS:HE3	1.21	1.43
1:B:330:PHE:CE2	1:B:333:GLU:HG3	1.55	1.40
1:A:706:HIS:CE1	1:A:738:LEU:CD2	2.06	1.37
1:A:489:CYS:SG	1:A:491:THR:CG2	2.16	1.33
1:A:79:LEU:CD1	1:A:98:ARG:CZ	2.10	1.27
1:A:717:MET:HE3	1:A:720:GLU:OE1	1.30	1.23
1:A:706:HIS:HE1	1:A:738:LEU:CD2	1.45	1.23
1:B:738:LEU:O	1:B:742:ARG:HG2	1.36	1.22
1:A:287:LEU:CD1	1:A:299:ALA:HB1	1.68	1.22
1:A:79:LEU:HD11	1:A:98:ARG:NE	1.56	1.21
1:A:515:LYS:NZ	1:A:519:LYS:CE	2.05	1.20
1:A:745:GLU:O	1:A:749:ARG:HG2	1.37	1.20
1:B:552:TYR:OH	1:B:583:ALA:HB2	1.44	1.17
1:A:296:TYR:CE1	1:A:300:LEU:CD1	2.33	1.11
1:A:740:TYR:O	1:A:743:VAL:HG22	1.47	1.11
1:A:128:ARG:NH2	1:A:163:GLU:HG2	1.63	1.10
1:A:287:LEU:HD11	1:A:299:ALA:HB1	1.16	1.10
2:D:5:U:H2'	2:D:6:C:H5''	1.24	1.10
2:D:9:U:H5'	2:D:10:A:OP2	1.52	1.08
1:A:128:ARG:HH21	1:A:163:GLU:HG2	0.90	1.06
1:A:79:LEU:CD1	1:A:98:ARG:NH2	2.12	1.06
1:B:559:PRO:HG2	1:B:590:ARG:NH2	1.71	1.06
1:B:599:PHE:HB3	1:B:622:ILE:HD11	1.23	1.06
1:B:651:GLU:OE1	1:B:688:ARG:NH2	1.89	1.06
2:D:9:U:H5''	2:D:10:A:H5'	1.35	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:717:MET:CE	1:A:720:GLU:OE1	2.03	1.06
1:A:128:ARG:HH21	1:A:163:GLU:CG	1.70	1.05
1:A:687:GLN:HE22	1:A:708:LEU:HD21	1.11	1.04
1:A:174:VAL:O	1:A:178:THR:HG23	1.56	1.03
1:B:738:LEU:CD1	1:B:742:ARG:HD3	1.88	1.01
1:B:753:PHE:CD2	1:B:783:GLN:HG3	1.96	1.01
1:B:632:ILE:HD11	2:C:14:A:C2	1.96	1.00
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:B:330:PHE:CD2	1:B:333:GLU:HG3	1.97	0.99
1:A:79:LEU:HD11	1:A:98:ARG:CZ	1.85	0.97
2:D:9:U:C5'	2:D:10:A:H5'	1.93	0.97
1:B:753:PHE:CE2	1:B:783:GLN:HA	1.98	0.97
1:A:687:GLN:NE2	1:A:708:LEU:HD21	1.79	0.97
1:A:296:TYR:HE1	1:A:300:LEU:HD11	1.15	0.97
1:B:330:PHE:CE2	1:B:333:GLU:CG	2.48	0.96
1:A:489:CYS:HG	1:A:491:THR:HG22	1.28	0.95
1:B:599:PHE:HB3	1:B:622:ILE:CD1	1.95	0.95
1:A:515:LYS:HZ1	1:A:519:LYS:CE	1.73	0.94
1:A:199:GLU:HG3	1:A:202:ARG:HH21	1.32	0.93
1:B:330:PHE:HE2	1:B:333:GLU:CG	1.82	0.92
1:A:86:HIS:NE2	1:A:90:THR:OG1	2.02	0.91
1:B:175:ARG:HA	2:D:1:G:H21	1.35	0.91
1:B:738:LEU:HD12	1:B:742:ARG:HD3	1.52	0.91
1:A:79:LEU:HD13	1:A:98:ARG:CZ	1.87	0.91
1:A:489:CYS:SG	1:A:491:THR:HG23	2.10	0.91
1:A:548:GLU:OE1	1:A:576:ARG:NH2	2.02	0.91
2:D:5:U:C2'	2:D:6:C:H5''	2.01	0.91
1:B:552:TYR:HH	1:B:583:ALA:HB2	1.36	0.90
2:D:9:U:C5'	2:D:10:A:OP2	2.19	0.90
1:B:175:ARG:HG2	2:D:1:G:N2	1.85	0.90
1:A:291:GLY:CA	1:A:324:THR:HG23	2.01	0.90
1:A:651:GLU:OE1	1:A:688:ARG:NH2	2.03	0.90
1:B:621:SER:HA	1:B:624:ARG:HG2	1.52	0.89
1:A:296:TYR:OH	1:A:337:CYS:HB2	1.72	0.89
1:B:594:PRO:HG2	1:B:599:PHE:CE2	2.07	0.89
1:B:559:PRO:HG2	1:B:590:ARG:HH21	1.32	0.89
1:A:431:GLY:HA3	2:D:8:U:O2'	1.73	0.89
1:B:552:TYR:OH	1:B:583:ALA:CB	2.20	0.89
1:B:279:CYS:SG	1:B:280:VAL:N	2.46	0.88
1:A:112:LYS:HD2	1:A:143:MET:CE	2.02	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:LEU:CD1	1:A:299:ALA:CB	2.52	0.88
1:A:79:LEU:HD13	1:A:98:ARG:HH21	1.34	0.88
1:A:295:ASN:OD1	1:A:298:GLU:HB2	1.74	0.88
1:A:119:HIS:HD2	1:A:122:TRP:CZ3	1.91	0.88
1:A:557:VAL:CG2	1:A:563:ILE:HD13	2.04	0.87
1:B:547:ILE:O	1:B:551:VAL:HG23	1.73	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	0.86
1:A:338:LEU:HD11	1:A:372:LEU:HG	1.54	0.86
1:A:685:GLU:OE2	1:A:688:ARG:NH1	2.07	0.86
1:B:660:SER:O	1:B:661:GLN:HB2	1.75	0.86
2:C:13:U:O2'	2:C:14:A:OP1	1.93	0.85
1:A:706:HIS:NE2	1:A:738:LEU:HD22	1.92	0.85
1:A:296:TYR:O	1:A:300:LEU:HG	1.75	0.85
1:B:558:PHE:CE1	1:B:590:ARG:NH2	2.45	0.85
1:B:558:PHE:HE1	1:B:590:ARG:NH2	1.75	0.84
1:B:664:LYS:O	1:B:665:PRO:O	1.95	0.84
1:A:706:HIS:NE2	1:A:738:LEU:CD2	2.41	0.84
1:B:657:LEU:HD22	1:B:663:MET:HB3	1.60	0.83
1:B:330:PHE:HE2	1:B:333:GLU:HG3	0.99	0.83
1:B:525:GLU:OE1	1:B:560:SER:OG	1.95	0.83
1:A:515:LYS:HZ3	1:A:519:LYS:CD	1.90	0.83
1:A:515:LYS:HZ3	1:A:519:LYS:CE	1.80	0.83
1:B:314:ASP:HA	1:B:317:THR:CG2	2.09	0.83
1:A:106:ASP:HB3	1:A:109:SER:HB2	1.59	0.83
1:A:175:ARG:HA	2:C:1:G:H21	1.44	0.83
1:A:315:ALA:O	1:A:319:ASN:ND2	2.12	0.82
1:B:314:ASP:HA	1:B:317:THR:HG21	1.60	0.82
1:A:717:MET:HE3	1:A:720:GLU:CD	1.98	0.82
1:A:287:LEU:HD12	1:A:287:LEU:O	1.80	0.82
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:B:289:VAL:O	1:B:293:ALA:HB2	1.78	0.81
1:A:632:ILE:CD1	2:D:14:A:C2	2.63	0.81
1:A:717:MET:CB	1:A:720:GLU:OE1	2.29	0.81
1:B:210:VAL:HG21	2:D:1:G:C6	2.16	0.80
1:B:86:HIS:CD2	1:B:87:PRO:HD2	2.14	0.80
1:B:175:ARG:HG2	2:D:1:G:C2	2.17	0.80
1:B:621:SER:O	1:B:625:SER:OG	1.98	0.80
2:D:6:C:C5'	2:D:6:C:H6	1.95	0.80
2:D:6:C:H5'	2:D:6:C:H6	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:738:LEU:HD11	1:B:742:ARG:HD3	1.63	0.79
1:A:83:ILE:HG23	1:A:91:LEU:HD11	1.65	0.79
1:A:375:GLN:N	1:A:375:GLN:OE1	2.15	0.78
1:B:279:CYS:SG	1:B:281:VAL:HG12	2.23	0.78
1:B:632:ILE:CD1	2:C:14:A:C2	2.66	0.78
1:B:558:PHE:HD1	1:B:559:PRO:HD2	1.47	0.78
1:A:717:MET:CE	1:A:720:GLU:CD	2.52	0.78
1:B:647:SER:OG	1:B:680:GLN:OE1	2.01	0.78
2:D:5:U:H2'	2:D:6:C:C5'	2.09	0.78
1:B:513:VAL:O	1:B:516:MET:HG2	1.84	0.77
2:C:12:U:OP1	2:C:12:U:H4'	1.85	0.77
1:A:738:LEU:HD23	1:A:742:ARG:HD3	1.65	0.77
1:A:738:LEU:O	1:A:742:ARG:HG2	1.85	0.77
1:B:331:PHE:HZ	1:B:371:ALA:HB3	1.49	0.77
2:D:5:U:O2'	2:D:6:C:OP1	2.03	0.76
1:B:531:LEU:HD23	1:B:547:ILE:HD11	1.68	0.76
1:B:550:GLU:OE1	1:B:550:GLU:HA	1.86	0.76
1:A:112:LYS:HD2	1:A:143:MET:HE3	1.68	0.76
1:A:651:GLU:CD	1:A:688:ARG:NH2	2.39	0.76
1:B:551:VAL:HG13	1:B:557:VAL:O	1.86	0.75
1:A:548:GLU:HA	1:A:551:VAL:HG12	1.67	0.75
1:B:594:PRO:HG2	1:B:599:PHE:HE2	1.52	0.75
1:B:660:SER:OG	1:B:663:MET:HB2	1.86	0.74
1:A:744:VAL:HB	1:A:779:ILE:HD11	1.69	0.74
2:C:13:U:H4'	2:C:14:A:OP2	1.87	0.74
1:A:354:ASN:O	1:A:358:THR:OG1	2.05	0.74
2:D:7:U:H5'	2:D:8:U:OP2	1.86	0.74
1:A:717:MET:HB3	1:A:720:GLU:OE1	1.87	0.74
1:A:710:GLY:C	2:D:18:C:O2'	2.25	0.73
1:A:744:VAL:O	1:A:748:CYS:HB2	1.88	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:86:HIS:HE2	1:A:90:THR:HG1	1.37	0.73
1:A:479:ASN:O	1:A:483:SER:OG	2.04	0.73
1:B:376:MET:HG2	1:B:381:PHE:CD2	2.24	0.73
1:B:558:PHE:CD1	1:B:559:PRO:HD2	2.23	0.72
1:B:559:PRO:CG	1:B:590:ARG:NH2	2.49	0.72
1:A:178:THR:HG21	1:A:211:THR:OG1	1.90	0.72
2:D:1:G:H3'	2:D:1:G:H8	1.54	0.72
1:B:314:ASP:CA	1:B:317:THR:CG2	2.67	0.72
2:D:9:U:C4'	2:D:10:A:OP2	2.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:SER:OG	1:A:663:MET:O	2.09	0.71
1:A:404:MET:HB3	1:A:426:MET:HE1	1.72	0.71
1:B:738:LEU:O	1:B:742:ARG:CG	2.28	0.71
1:A:79:LEU:CD1	1:A:98:ARG:NE	2.34	0.71
2:D:9:U:H5''	2:D:10:A:C5'	2.19	0.70
1:A:112:LYS:HD2	1:A:143:MET:HE1	1.72	0.70
1:B:280:VAL:O	1:B:284:ASN:ND2	2.24	0.70
1:A:515:LYS:NZ	1:A:519:LYS:CD	2.52	0.70
1:A:106:ASP:CB	1:A:109:SER:HB2	2.22	0.69
1:A:498:ASN:O	1:A:501:SER:OG	2.08	0.69
1:A:341:MET:CE	1:A:348:PRO:HG3	2.23	0.68
1:A:447:ARG:HH22	1:A:477:MET:HE1	1.58	0.68
1:A:296:TYR:CZ	1:A:300:LEU:HD21	2.28	0.68
1:A:431:GLY:CA	2:D:8:U:O2'	2.41	0.68
1:A:705:TYR:O	1:A:709:VAL:HG23	1.93	0.68
1:B:753:PHE:CG	1:B:783:GLN:HG3	2.27	0.68
1:A:283:TYR:OH	1:A:309:ASN:ND2	2.27	0.68
1:A:609:ASN:HB2	1:A:611:MET:HG3	1.76	0.68
1:A:666:ASP:O	1:A:669:SER:HB2	1.93	0.68
1:B:757:ARG:NH2	1:B:783:GLN:OE1	2.26	0.68
1:B:209:LEU:O	1:B:213:ASN:ND2	2.27	0.68
1:A:565:ARG:NH2	1:A:595:ASP:OD2	2.26	0.67
1:A:717:MET:HB2	1:A:720:GLU:OE1	1.91	0.67
1:B:314:ASP:C	1:B:317:THR:CG2	2.62	0.67
1:B:376:MET:CE	1:B:381:PHE:CE2	2.78	0.67
2:D:1:G:C8	2:D:1:G:H3'	2.30	0.66
1:A:456:ASP:O	1:A:460:THR:HG23	1.95	0.66
2:D:14:A:O2'	2:D:15:U:OP1	2.13	0.66
1:A:200:LEU:HD23	1:A:200:LEU:C	2.15	0.66
1:A:284:ASN:O	1:A:320:GLU:OE1	2.13	0.66
1:B:88:LEU:N	1:B:89:PRO:HD2	2.10	0.66
1:A:717:MET:HE2	1:A:720:GLU:HG3	1.78	0.66
1:A:119:HIS:CD2	1:A:122:TRP:CZ3	2.81	0.66
1:B:651:GLU:CD	1:B:688:ARG:NH2	2.50	0.66
2:D:12:U:H6	2:D:12:U:O5'	1.78	0.65
1:B:379:THR:OG1	1:B:379:THR:O	2.12	0.65
1:A:150:ARG:HG2	1:A:150:ARG:HH11	1.61	0.65
1:A:760:LEU:HD22	1:A:779:ILE:HG13	1.79	0.65
1:A:357:MET:HG2	1:A:369:ALA:HB1	1.79	0.65
1:A:175:ARG:HA	2:C:1:G:N2	2.11	0.65
1:A:661:GLN:OE1	1:B:384:ASN:OD1	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:VAL:O	1:B:178:THR:HG23	1.96	0.65
1:B:565:ARG:NH2	1:B:595:ASP:OD2	2.30	0.65
1:B:577:LEU:HD21	1:B:611:MET:CE	2.26	0.65
1:B:260:LEU:HB3	1:B:263:GLU:HG2	1.79	0.65
1:A:631:LEU:HD13	1:A:666:ASP:HB2	1.79	0.65
1:A:760:LEU:C	1:A:760:LEU:HD12	2.16	0.64
1:A:721:ALA:O	1:A:725:ILE:HG13	1.97	0.64
1:A:419:ASN:HD22	1:A:419:ASN:H	1.44	0.64
1:A:419:ASN:ND2	1:A:422:THR:H	1.96	0.64
1:A:651:GLU:OE2	1:A:688:ARG:NH2	2.30	0.64
1:A:743:VAL:O	1:A:747:TYR:HB2	1.97	0.64
2:C:12:U:C5	2:C:14:A:C2	2.85	0.64
1:A:111:LEU:HD13	1:A:144:VAL:HG23	1.79	0.64
1:A:738:LEU:CD2	1:A:742:ARG:HD3	2.28	0.64
1:A:675:ASN:ND2	2:D:17:U:H5'	2.12	0.64
1:A:706:HIS:NE2	1:A:738:LEU:HD23	2.13	0.64
1:B:559:PRO:HD2	1:B:590:ARG:HH22	1.63	0.64
1:A:178:THR:CG2	1:A:211:THR:OG1	2.46	0.63
1:A:557:VAL:HG21	1:A:563:ILE:HD13	1.81	0.63
1:A:338:LEU:HD22	1:A:375:GLN:HG2	1.80	0.63
1:B:201:ARG:NH2	1:B:235:GLU:OE1	2.28	0.63
1:A:662:THR:HG21	1:B:386:ASN:HB3	1.81	0.63
2:D:9:U:H5'	2:D:10:A:H5'	1.78	0.63
1:B:583:ALA:O	1:B:587:VAL:HG23	1.99	0.63
1:A:634:TYR:O	1:A:638:MET:HG3	1.98	0.63
1:B:651:GLU:CD	1:B:688:ARG:HH22	2.03	0.63
1:A:338:LEU:HD11	1:A:372:LEU:CG	2.27	0.63
1:A:477:MET:HE1	1:A:480:GLU:OE2	1.97	0.63
1:A:163:GLU:HG3	1:A:164:THR:N	2.13	0.62
1:A:419:ASN:ND2	1:A:419:ASN:H	1.98	0.62
1:B:376:MET:HE1	1:B:381:PHE:CE2	2.34	0.62
1:B:481:MET:HE1	1:B:492:THR:HG21	1.80	0.62
1:B:174:VAL:HG22	1:B:205:VAL:CG1	2.30	0.62
1:B:666:ASP:O	1:B:669:SER:N	2.31	0.62
1:A:447:ARG:NH2	1:A:477:MET:HE1	2.15	0.62
1:A:260:LEU:HB3	1:A:263:GLU:CG	2.29	0.62
1:A:532:LEU:HD13	1:A:547:ILE:HD12	1.80	0.62
1:A:740:TYR:C	1:A:743:VAL:HG22	2.18	0.62
1:A:516:MET:O	1:A:521:PHE:HB2	2.00	0.62
1:A:338:LEU:CD2	1:A:375:GLN:CB	2.78	0.61
1:A:401:PHE:HE1	1:A:429:VAL:HG21	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:TYR:HE1	1:A:586:GLU:HG3	1.66	0.61
1:B:279:CYS:SG	1:B:281:VAL:CG1	2.87	0.61
1:A:557:VAL:HG23	1:A:563:ILE:CD1	2.30	0.61
1:A:79:LEU:HD11	1:A:98:ARG:HE	1.63	0.61
1:A:349:ASN:OD1	1:A:349:ASN:N	2.33	0.61
1:A:419:ASN:ND2	1:A:422:THR:OG1	2.34	0.61
1:A:142:GLU:HG3	1:A:172:LEU:HD23	1.81	0.60
1:B:494:ASN:OD1	1:B:527:SER:OG	2.15	0.60
1:A:407:MET:O	1:A:411:MET:HG3	2.00	0.60
1:A:632:ILE:HD11	2:D:14:A:C2	2.36	0.60
1:A:147:ALA:O	1:A:151:GLU:N	2.34	0.60
1:A:366:VAL:HG12	1:A:394:MET:HE3	1.83	0.60
1:A:543:GLY:O	1:A:547:ILE:HG13	2.00	0.60
1:A:700:PRO:HB3	1:A:704:THR:HG21	1.82	0.60
1:A:98:ARG:HH21	1:A:101:GLU:CD	2.05	0.60
1:B:595:ASP:N	1:B:595:ASP:OD1	2.25	0.60
1:B:717:MET:O	1:B:720:GLU:HG2	2.01	0.60
1:A:740:TYR:O	1:A:743:VAL:CG2	2.36	0.60
1:B:757:ARG:NH2	1:B:780:GLU:OE1	2.33	0.60
1:A:660:SER:O	1:A:662:THR:HG22	2.02	0.60
1:A:548:GLU:CA	1:A:551:VAL:HG12	2.31	0.60
1:A:745:GLU:HA	1:A:778:TYR:OH	2.01	0.60
1:B:657:LEU:HD22	1:B:663:MET:CB	2.29	0.60
1:A:219:TYR:CE1	1:A:228:ARG:HD2	2.37	0.60
1:A:489:CYS:SG	1:A:490:ILE:N	2.75	0.60
1:B:246:PHE:O	1:B:250:THR:OG1	2.06	0.60
1:A:128:ARG:NE	1:A:163:GLU:OE1	2.32	0.59
1:A:477:MET:CE	1:A:480:GLU:OE2	2.49	0.59
1:B:654:LEU:HD23	1:B:658:LYS:HE3	1.84	0.59
1:B:94:PHE:O	1:B:97:SER:OG	2.18	0.59
1:B:73:SER:O	1:B:77:GLN:HG3	2.02	0.59
1:A:757:ARG:O	1:A:760:LEU:HG	2.03	0.59
1:B:577:LEU:HD13	1:B:605:ILE:HG13	1.84	0.59
1:A:284:ASN:ND2	1:A:316:VAL:HG13	2.18	0.59
1:A:711:GLY:N	2:D:18:C:O2'	2.36	0.59
1:A:738:LEU:O	1:A:742:ARG:CG	2.51	0.59
1:A:111:LEU:HD13	1:A:144:VAL:CG2	2.32	0.58
1:A:548:GLU:HA	1:A:551:VAL:CG1	2.33	0.58
1:B:289:VAL:O	1:B:293:ALA:CB	2.49	0.58
1:A:296:TYR:O	1:A:300:LEU:CG	2.49	0.58
1:A:515:LYS:HZ1	1:A:519:LYS:HE3	0.77	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:575:ARG:CD	1:B:605:ILE:HD13	2.33	0.58
1:B:630:ASP:OD1	1:B:631:LEU:N	2.35	0.58
1:A:260:LEU:HB3	1:A:263:GLU:HG3	1.85	0.58
1:A:446:MET:O	1:A:451:VAL:HG12	2.02	0.58
1:A:489:CYS:SG	1:A:491:THR:N	2.76	0.58
1:B:560:SER:OG	1:B:562:VAL:HG23	2.04	0.58
2:D:1:G:C8	2:D:1:G:C3'	2.86	0.58
1:A:660:SER:C	1:A:662:THR:H	2.08	0.58
1:B:577:LEU:HD21	1:B:611:MET:HE1	1.85	0.58
1:B:175:ARG:HA	2:D:1:G:N2	2.14	0.57
1:A:432:LYS:HG2	1:A:433:ARG:N	2.14	0.57
1:B:168:PRO:O	1:B:169:GLY:O	2.21	0.57
1:A:519:LYS:HB3	1:A:521:PHE:CD2	2.39	0.57
1:A:712:TYR:O	1:A:717:MET:O	2.22	0.57
1:B:459:ASN:OD1	1:B:492:THR:HG22	2.03	0.57
1:A:246:PHE:O	1:A:250:THR:OG1	2.14	0.57
1:B:284:ASN:N	1:B:284:ASN:HD22	2.01	0.57
1:A:429:VAL:O	1:A:467:ARG:NH1	2.30	0.57
1:A:86:HIS:CD2	1:A:87:PRO:O	2.57	0.57
2:D:6:C:C6	2:D:6:C:H5'	2.36	0.57
1:A:668:VAL:O	1:A:672:THR:OG1	2.17	0.57
1:B:666:ASP:O	1:B:668:VAL:N	2.38	0.57
2:D:9:U:H4'	2:D:10:A:OP2	2.05	0.57
1:A:631:LEU:CD1	1:A:666:ASP:HB2	2.34	0.56
1:B:292:LYS:HA	1:B:327:ARG:HD3	1.86	0.56
1:B:314:ASP:C	1:B:317:THR:HG22	2.25	0.56
1:A:519:LYS:HB3	1:A:521:PHE:CE2	2.41	0.56
1:A:744:VAL:HG23	1:A:745:GLU:N	2.20	0.56
1:B:540:ASN:OD1	1:B:543:GLY:N	2.33	0.56
1:B:167:PRO:HB2	1:B:168:PRO:HD2	1.88	0.56
1:B:376:MET:HE1	1:B:381:PHE:CZ	2.41	0.56
1:B:367:ASP:OD2	1:B:400:ARG:NH1	2.38	0.56
1:A:353:TYR:HE2	1:A:381:PHE:HD2	1.54	0.56
1:A:753:PHE:O	1:A:756:ALA:HB3	2.06	0.56
1:B:660:SER:C	1:B:662:THR:H	2.09	0.56
1:B:773:LYS:N	1:B:776:GLU:OE1	2.39	0.56
1:A:291:GLY:HA2	1:A:324:THR:CG2	2.29	0.56
1:B:459:ASN:CG	1:B:492:THR:HG22	2.27	0.55
1:A:86:HIS:HD2	1:A:87:PRO:O	1.90	0.55
1:A:377:LYS:C	1:A:379:THR:H	2.09	0.55
1:B:657:LEU:CD2	1:B:663:MET:HG3	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:ILE:HD13	2:D:14:A:C2	2.42	0.55
1:A:200:LEU:HD23	1:A:201:ARG:N	2.21	0.55
1:A:231:ALA:O	1:A:235:GLU:HG3	2.07	0.55
1:A:284:ASN:ND2	1:A:316:VAL:CG1	2.70	0.55
1:B:114:LEU:HD22	1:B:122:TRP:HB3	1.88	0.55
1:A:668:VAL:HG13	2:D:16:U:C2	2.42	0.55
1:A:340:THR:C	1:A:342:ALA:H	2.09	0.55
1:A:745:GLU:O	1:A:749:ARG:CG	2.32	0.55
1:B:594:PRO:HG2	1:B:599:PHE:CZ	2.41	0.55
1:A:754:GLU:HA	1:A:757:ARG:HE	1.71	0.55
1:B:599:PHE:CD1	1:B:622:ILE:HG12	2.42	0.54
1:A:571:ASN:HB3	1:A:580:MET:HG3	1.89	0.54
1:A:706:HIS:HE1	1:A:738:LEU:CG	2.18	0.54
1:A:270:ASP:O	1:A:274:ARG:HG3	2.07	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:A:745:GLU:HA	1:A:778:TYR:CZ	2.43	0.54
1:A:76:ALA:O	1:A:79:LEU:N	2.40	0.54
1:A:706:HIS:CE1	1:A:738:LEU:HD23	2.30	0.54
1:A:717:MET:HE2	1:A:720:GLU:CG	2.38	0.54
1:B:178:THR:HG21	1:B:211:THR:OG1	2.07	0.54
1:B:379:THR:O	1:B:381:PHE:N	2.36	0.54
1:A:280:VAL:HG23	1:A:281:VAL:H	1.71	0.54
1:A:296:TYR:HH	1:A:337:CYS:HB2	1.72	0.54
1:B:577:LEU:HD22	1:B:609:ASN:HD22	1.73	0.54
1:A:353:TYR:CE2	1:A:381:PHE:HD2	2.26	0.54
1:A:582:THR:O	1:A:585:GLN:HB3	2.08	0.54
1:A:725:ILE:C	1:A:727:TYR:H	2.12	0.54
1:B:586:GLU:O	1:B:590:ARG:HG3	2.08	0.54
1:A:715:LEU:C	1:A:717:MET:HG2	2.27	0.53
1:A:286:LEU:HD12	1:A:286:LEU:O	2.07	0.53
1:A:353:TYR:HE2	1:A:381:PHE:CD2	2.26	0.53
1:A:316:VAL:HG23	2:C:5:U:C2	2.43	0.53
1:A:718:PHE:CG	1:A:747:TYR:CE1	2.97	0.53
1:B:167:PRO:O	1:B:170:SER:OG	2.17	0.53
1:B:174:VAL:HG22	1:B:205:VAL:HG12	1.90	0.53
1:B:580:MET:HG2	1:B:602:MET:HE2	1.89	0.53
1:A:174:VAL:HG21	1:A:208:THR:HG23	1.89	0.53
1:A:717:MET:HE2	1:A:720:GLU:CD	2.28	0.53
1:A:399:SER:OG	1:A:432:LYS:HE3	2.08	0.53
1:B:330:PHE:CD2	1:B:333:GLU:CG	2.81	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:596:LEU:HD21	1:B:630:ASP:HB2	1.90	0.53
1:B:631:LEU:O	1:B:635:ASN:N	2.41	0.53
1:A:504:GLY:O	1:A:506:TRP:N	2.41	0.53
1:A:718:PHE:CD1	1:A:747:TYR:CE1	2.97	0.53
1:B:306:MET:HE1	1:B:317:THR:HG21	1.91	0.52
1:B:88:LEU:N	1:B:89:PRO:CD	2.72	0.52
1:B:602:MET:O	1:B:605:ILE:HG22	2.10	0.52
1:A:635:ASN:OD1	1:A:669:SER:OG	2.14	0.52
1:A:88:LEU:HB3	1:A:89:PRO:HD3	1.92	0.52
2:D:7:U:H2'	2:D:7:U:O2	2.09	0.52
1:B:298:GLU:C	1:B:300:LEU:H	2.12	0.52
1:B:688:ARG:O	1:B:691:SER:OG	2.26	0.52
1:A:698:MET:O	1:A:700:PRO:HD3	2.09	0.52
1:A:460:THR:OG1	1:A:461:LEU:N	2.42	0.52
1:B:715:LEU:O	1:B:716:GLU:C	2.48	0.52
1:B:408:LEU:HD13	1:B:426:MET:SD	2.49	0.52
1:A:150:ARG:HG2	1:A:150:ARG:NH1	2.24	0.52
1:B:666:ASP:O	1:B:667:VAL:C	2.45	0.52
2:C:13:U:OP1	2:C:13:U:H3'	2.10	0.52
1:A:119:HIS:HD2	1:A:122:TRP:CE3	2.28	0.51
1:A:754:GLU:C	1:A:756:ALA:H	2.12	0.51
1:A:79:LEU:HD12	1:A:98:ARG:CZ	2.30	0.51
1:A:661:GLN:O	1:B:354:ASN:ND2	2.44	0.51
1:B:724:VAL:O	1:B:727:TYR:N	2.43	0.51
1:A:742:ARG:NH1	2:D:18:C:C2	2.79	0.51
1:B:635:ASN:ND2	1:B:669:SER:OG	2.30	0.51
2:D:13:U:H3'	2:D:13:U:H6	1.75	0.51
1:B:253:ALA:O	1:B:257:ARG:HG3	2.11	0.51
1:B:685:GLU:OE1	1:B:688:ARG:NH1	2.44	0.51
1:B:86:HIS:CD2	1:B:87:PRO:CD	2.89	0.51
1:B:323:GLY:O	1:B:327:ARG:HG2	2.10	0.51
1:B:599:PHE:CB	1:B:622:ILE:CD1	2.81	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:A:683:VAL:HB	1:A:712:TYR:CE1	2.46	0.50
1:B:432:LYS:HG2	1:B:433:ARG:H	1.75	0.50
1:B:657:LEU:CD2	1:B:663:MET:CB	2.88	0.50
1:A:371:ALA:O	1:A:375:GLN:OE1	2.30	0.50
1:A:510:GLN:O	1:A:512:ILE:N	2.44	0.50
1:A:740:TYR:HA	1:A:743:VAL:HG22	1.94	0.50
1:B:564:LEU:O	1:B:568:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:GLU:CG	1:A:172:LEU:HD23	2.41	0.50
1:B:529:SER:O	1:B:533:GLN:HG3	2.12	0.50
1:B:575:ARG:HD2	1:B:605:ILE:HD13	1.93	0.50
1:A:557:VAL:HG22	1:A:563:ILE:HD13	1.90	0.50
1:A:739:THR:O	1:A:742:ARG:HG2	2.11	0.50
2:D:12:U:H4'	2:D:14:A:H5''	1.93	0.50
2:D:6:C:C5'	2:D:6:C:C6	2.85	0.50
1:A:106:ASP:HB3	1:A:109:SER:CB	2.36	0.50
1:A:548:GLU:C	1:A:551:VAL:HG12	2.32	0.50
1:A:718:PHE:CG	1:A:747:TYR:CZ	3.01	0.49
1:B:217:ASP:O	1:B:221:ARG:HG3	2.12	0.49
1:A:221:ARG:NH1	1:B:433:ARG:HD3	2.27	0.49
1:B:528:TYR:O	1:B:532:LEU:HD13	2.12	0.49
1:A:586:GLU:O	1:A:590:ARG:N	2.30	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:741:ARG:O	1:B:745:GLU:HG2	2.13	0.49
1:B:599:PHE:CG	1:B:622:ILE:HG12	2.47	0.49
1:A:401:PHE:CE1	1:A:429:VAL:HG21	2.45	0.49
1:A:743:VAL:HG23	1:A:744:VAL:N	2.28	0.49
1:A:775:LEU:O	1:A:777:ALA:N	2.46	0.49
1:A:456:ASP:O	1:A:460:THR:CG2	2.59	0.49
1:B:161:LEU:HD13	1:B:180:VAL:HG11	1.95	0.49
1:B:209:LEU:HG	1:B:213:ASN:HD21	1.77	0.49
1:B:423:TRP:CD2	1:B:446:MET:HG3	2.47	0.49
1:B:552:TYR:OH	1:B:583:ALA:CA	2.59	0.49
1:A:419:ASN:ND2	1:A:419:ASN:N	2.55	0.49
1:B:525:GLU:OE1	1:B:560:SER:CB	2.61	0.49
1:A:443:LEU:HD22	1:A:461:LEU:HD22	1.95	0.48
1:A:753:PHE:O	1:A:756:ALA:N	2.43	0.48
1:B:107:ILE:HD12	1:B:107:ILE:H	1.78	0.48
1:B:413:ARG:HG3	1:B:413:ARG:O	2.13	0.48
1:A:174:VAL:O	1:A:178:THR:CG2	2.45	0.48
1:B:106:ASP:HB3	1:B:109:SER:HB3	1.95	0.48
1:A:744:VAL:CG2	1:A:745:GLU:N	2.76	0.48
1:B:243:PRO:HB3	1:B:247:THR:HG21	1.95	0.48
1:B:745:GLU:O	1:B:749:ARG:HG3	2.14	0.48
1:B:660:SER:OG	1:B:663:MET:N	2.45	0.48
1:A:657:LEU:O	1:A:665:PRO:HD3	2.14	0.48
1:A:677:PHE:O	1:A:681:GLY:N	2.46	0.48
1:B:558:PHE:CD1	1:B:559:PRO:CD	2.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:12:U:H4'	2:D:14:A:C5'	2.44	0.48
1:A:106:ASP:CG	1:A:109:SER:HB2	2.34	0.48
1:A:419:ASN:HD22	1:A:422:THR:H	1.60	0.48
1:B:330:PHE:CD2	1:B:333:GLU:HB2	2.48	0.48
1:A:641:TYR:HB3	1:A:646:GLU:O	2.13	0.47
1:A:124:LEU:O	1:A:128:ARG:HG3	2.14	0.47
1:A:432:LYS:CG	1:A:433:ARG:H	2.16	0.47
1:B:375:GLN:O	1:B:379:THR:HG23	2.13	0.47
1:A:98:ARG:NH2	1:A:101:GLU:OE2	2.47	0.47
1:A:609:ASN:N	1:A:609:ASN:OD1	2.47	0.47
1:A:690:LEU:O	1:A:694:VAL:HG23	2.14	0.47
1:A:736:MET:HG3	1:A:739:THR:OG1	2.14	0.47
1:B:287:LEU:CD1	1:B:317:THR:OG1	2.62	0.47
1:B:565:ARG:O	1:B:569:ILE:HG13	2.14	0.47
1:A:497:LEU:HB2	1:A:530:LEU:HD23	1.97	0.47
1:B:352:THR:O	1:B:356:VAL:HG23	2.14	0.47
1:A:431:GLY:N	2:D:8:U:O2'	2.48	0.47
1:A:116:LEU:HG	1:A:116:LEU:O	2.13	0.47
1:A:632:ILE:HD11	2:D:14:A:N1	2.30	0.47
1:A:510:GLN:O	1:A:513:VAL:HG12	2.14	0.47
1:A:738:LEU:HD23	1:A:738:LEU:O	2.15	0.47
1:A:760:LEU:HD12	1:A:761:SER:N	2.30	0.47
1:B:399:SER:OG	1:B:430:SER:O	2.32	0.47
1:B:623:LYS:O	1:B:626:GLY:N	2.30	0.47
1:B:604:SER:OG	1:B:636:SER:HB3	2.15	0.47
1:A:287:LEU:HD13	1:A:299:ALA:HB1	1.78	0.47
1:B:161:LEU:CD1	1:B:180:VAL:HG11	2.44	0.47
1:A:106:ASP:O	1:A:109:SER:HB2	2.14	0.47
1:A:374:ASP:O	1:A:378:LYS:HD2	2.15	0.47
1:A:742:ARG:NH1	2:D:18:C:N1	2.62	0.47
1:A:98:ARG:O	1:A:102:LEU:HG	2.15	0.47
1:A:141:LEU:CD2	1:A:166:LEU:HD11	2.45	0.46
1:B:284:ASN:N	1:B:284:ASN:ND2	2.63	0.46
1:B:659:CYS:O	1:B:661:GLN:N	2.48	0.46
1:A:313:PRO:HB3	1:A:317:THR:HG21	1.96	0.46
1:A:560:SER:O	1:A:561:TRP:C	2.53	0.46
1:B:453:LEU:H	1:B:453:LEU:HD12	1.80	0.46
1:A:338:LEU:CD2	1:A:375:GLN:HB3	2.45	0.46
1:A:314:ASP:OD1	1:A:317:THR:OG1	2.34	0.46
1:A:307:GLU:O	1:A:310:GLY:N	2.48	0.46
1:A:742:ARG:NH1	2:D:18:C:C6	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:TYR:HB3	1:B:365:LYS:O	2.15	0.46
1:B:606:TYR:O	1:B:611:MET:O	2.33	0.46
1:A:515:LYS:NZ	1:A:519:LYS:HD3	2.31	0.46
1:A:526:GLN:OE1	1:A:526:GLN:N	2.28	0.46
2:D:14:A:H3'	2:D:14:A:C8	2.51	0.46
1:B:513:VAL:HA	1:B:516:MET:SD	2.55	0.46
2:D:13:U:C6	2:D:13:U:C3'	2.99	0.46
1:A:129:TRP:CZ2	1:A:133:GLU:OE1	2.69	0.46
1:A:660:SER:OG	1:A:663:MET:N	2.45	0.46
1:B:298:GLU:C	1:B:300:LEU:N	2.69	0.46
1:B:446:MET:HB2	1:B:446:MET:HE2	1.75	0.46
1:B:577:LEU:CD2	1:B:611:MET:CE	2.93	0.46
1:A:548:GLU:HB3	1:A:552:TYR:CE2	2.51	0.46
1:B:283:TYR:CD1	1:B:306:MET:HA	2.51	0.46
1:B:575:ARG:HD3	1:B:605:ILE:HD13	1.97	0.46
1:A:119:HIS:CD2	1:A:122:TRP:CE3	3.03	0.46
1:A:296:TYR:CE1	1:A:300:LEU:HD21	2.51	0.46
1:A:594:PRO:HG2	1:A:599:PHE:CZ	2.51	0.46
1:A:571:ASN:O	1:A:576:ARG:N	2.37	0.45
1:B:161:LEU:HD13	1:B:180:VAL:CG1	2.46	0.45
1:B:376:MET:CE	1:B:381:PHE:CZ	2.98	0.45
1:B:490:ILE:HG22	1:B:494:ASN:HD21	1.80	0.45
1:B:559:PRO:HB2	1:B:564:LEU:HD21	1.97	0.45
1:A:212:TYR:CD1	1:A:236:MET:HB3	2.51	0.45
1:B:283:TYR:O	1:B:287:LEU:HB2	2.16	0.45
1:A:237:ARG:CZ	1:A:274:ARG:NH1	2.80	0.45
1:A:740:TYR:CA	1:A:743:VAL:HG22	2.45	0.45
1:B:501:SER:HA	1:B:534:CYS:SG	2.57	0.45
1:B:277:ALA:HA	1:B:278:PRO:HD2	1.81	0.45
1:B:331:PHE:HZ	1:B:371:ALA:CB	2.26	0.45
1:B:752:ARG:HG2	1:B:752:ARG:H	1.57	0.45
1:A:141:LEU:HD23	1:A:172:LEU:HD21	1.99	0.45
1:A:200:LEU:O	1:A:205:VAL:HB	2.15	0.45
1:A:86:HIS:CG	1:A:87:PRO:HD2	2.52	0.45
1:B:127:LEU:HD11	1:B:141:LEU:HA	1.97	0.45
1:B:743:VAL:O	1:B:747:TYR:HB2	2.17	0.45
1:A:291:GLY:HA3	1:A:324:THR:HG23	1.94	0.45
1:A:348:PRO:O	1:A:381:PHE:CE2	2.70	0.45
1:B:197:PHE:O	1:B:200:LEU:HB3	2.16	0.45
1:A:161:LEU:HD22	1:A:184:LEU:HD21	1.98	0.45
1:B:368:GLU:N	1:B:368:GLU:OE1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:VAL:HG13	1:A:451:VAL:O	2.17	0.45
1:A:668:VAL:HG13	2:D:16:U:N1	2.32	0.45
1:A:715:LEU:HB3	1:A:717:MET:CG	2.47	0.45
1:B:455:ARG:NE	1:B:489:CYS:SG	2.90	0.45
1:B:562:VAL:HG23	1:B:563:ILE:H	1.81	0.45
1:B:175:ARG:CG	2:D:1:G:N2	2.70	0.45
1:A:610:GLY:O	1:A:612:TYR:N	2.48	0.44
1:B:594:PRO:CG	1:B:599:PHE:CE2	2.91	0.44
1:B:660:SER:C	1:B:662:THR:N	2.70	0.44
2:D:10:A:H8	2:D:10:A:OP2	2.00	0.44
1:A:441:ARG:HD3	1:A:441:ARG:HA	1.77	0.44
1:A:513:VAL:HG23	1:A:516:MET:HE3	1.98	0.44
1:A:653:ILE:HA	1:A:656:GLN:HB2	1.98	0.44
1:A:271:LEU:HD12	1:A:271:LEU:HA	1.85	0.44
1:A:268:PHE:CD2	1:A:286:LEU:HD22	2.52	0.44
1:B:654:LEU:CD2	1:B:658:LYS:HE3	2.46	0.44
1:A:777:ALA:O	1:A:781:ASP:N	2.49	0.44
1:B:219:TYR:HA	1:B:222:MET:HE2	1.99	0.44
1:B:314:ASP:C	1:B:317:THR:HG23	2.35	0.44
1:B:306:MET:CE	1:B:317:THR:HG21	2.46	0.44
1:B:660:SER:O	1:B:662:THR:N	2.50	0.44
1:B:661:GLN:HE21	1:B:661:GLN:HB3	1.53	0.44
2:D:13:U:C6	2:D:13:U:H3'	2.52	0.44
1:A:142:GLU:HG3	1:A:172:LEU:CD2	2.46	0.44
1:B:116:LEU:HD23	1:B:116:LEU:HA	1.77	0.44
1:B:400:ARG:O	1:B:404:MET:HG3	2.18	0.44
1:A:112:LYS:CD	1:A:143:MET:HE3	2.43	0.44
1:A:341:MET:HE2	1:A:348:PRO:HG3	1.94	0.44
1:A:387:THR:O	1:A:391:VAL:HG23	2.17	0.44
1:A:643:LYS:HA	1:A:643:LYS:HD2	1.69	0.44
1:A:709:VAL:HG13	1:A:721:ALA:HB1	1.99	0.44
1:B:211:THR:O	1:B:215:VAL:HG23	2.18	0.44
1:A:706:HIS:CD2	1:A:706:HIS:O	2.70	0.44
1:A:83:ILE:H	1:A:83:ILE:HG13	1.59	0.44
1:A:338:LEU:CD2	1:A:375:GLN:HG2	2.46	0.44
2:D:14:A:H3'	2:D:14:A:H8	1.82	0.44
1:B:490:ILE:HG22	1:B:494:ASN:ND2	2.33	0.44
1:A:652:LYS:HD3	1:A:652:LYS:HA	1.72	0.43
1:A:692:GLU:HA	1:A:695:ALA:HB3	1.99	0.43
1:A:706:HIS:CE1	1:A:738:LEU:HB3	2.53	0.43
1:B:614:LYS:O	1:B:617:GLU:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:LEU:HD22	1:A:375:GLN:CG	2.48	0.43
1:A:548:GLU:HB3	1:A:552:TYR:HE2	1.82	0.43
1:A:684:LYS:HG3	1:A:685:GLU:N	2.32	0.43
1:A:687:GLN:HE21	1:A:708:LEU:HD11	1.83	0.43
1:A:338:LEU:HD21	1:A:375:GLN:CB	2.48	0.43
1:A:377:LYS:C	1:A:379:THR:N	2.72	0.43
1:A:578:ASP:N	1:A:578:ASP:OD1	2.49	0.43
1:A:754:GLU:C	1:A:756:ALA:N	2.71	0.43
1:B:577:LEU:HD22	1:B:609:ASN:ND2	2.32	0.43
1:A:348:PRO:O	1:A:381:PHE:CZ	2.72	0.43
1:A:655:ASN:HA	1:A:658:LYS:HE3	2.00	0.43
1:A:341:MET:HE3	1:A:348:PRO:HG3	1.99	0.43
1:A:701:CYS:H	1:A:704:THR:HG1	1.66	0.43
1:B:415:GLY:O	1:B:417:THR:N	2.52	0.43
1:A:761:SER:C	1:A:763:VAL:H	2.22	0.43
1:B:114:LEU:HD22	1:B:122:TRP:CB	2.49	0.43
2:D:6:C:C6	2:D:6:C:C4'	3.02	0.43
1:A:270:ASP:O	1:A:274:ARG:CG	2.66	0.43
1:B:298:GLU:O	1:B:300:LEU:N	2.52	0.43
1:B:666:ASP:C	1:B:668:VAL:N	2.69	0.43
1:B:519:LYS:HB3	1:B:521:PHE:CD2	2.54	0.42
1:A:287:LEU:HD13	1:A:299:ALA:CB	2.40	0.42
1:A:612:TYR:HA	1:A:640:MET:HE1	2.01	0.42
1:B:581:GLU:O	1:B:582:THR:C	2.57	0.42
1:A:619:PHE:O	1:A:622:ILE:HB	2.18	0.42
1:A:634:TYR:HB3	1:A:657:LEU:HD11	2.01	0.42
1:B:659:CYS:C	1:B:661:GLN:N	2.71	0.42
1:B:709:VAL:O	1:B:713:SER:OG	2.25	0.42
1:A:253:ALA:O	1:A:257:ARG:HG3	2.19	0.42
1:A:303:LEU:HA	1:A:303:LEU:HD23	1.92	0.42
1:A:95:LEU:HD22	1:A:126:LEU:HD13	2.01	0.42
1:B:575:ARG:HD3	1:B:575:ARG:HA	1.66	0.42
1:B:559:PRO:CD	1:B:590:ARG:HH22	2.30	0.42
1:A:431:GLY:O	1:A:432:LYS:HB2	2.18	0.42
1:A:692:GLU:O	1:A:695:ALA:N	2.53	0.42
1:B:172:LEU:HB2	1:B:177:TYR:CE2	2.54	0.42
1:B:314:ASP:O	1:B:317:THR:HG23	2.20	0.42
1:B:667:VAL:HA	1:B:670:TYR:HD2	1.85	0.42
1:B:676:GLY:O	1:B:680:GLN:HG3	2.19	0.42
1:A:173:ASP:O	1:A:177:TYR:HD2	2.02	0.42
1:A:300:LEU:HD23	1:A:321:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:725:ILE:C	1:A:727:TYR:N	2.73	0.42
1:B:441:ARG:HA	1:B:441:ARG:HD3	1.74	0.42
1:B:654:LEU:O	1:B:657:LEU:HB2	2.19	0.42
1:A:243:PRO:HB3	1:A:247:THR:HG21	2.01	0.42
1:A:500:LEU:HD22	1:A:505:ASP:HB3	2.02	0.42
1:A:560:SER:O	1:A:563:ILE:N	2.53	0.42
1:B:178:THR:CG2	1:B:211:THR:OG1	2.67	0.42
1:B:715:LEU:HD12	1:B:717:MET:CE	2.49	0.42
1:B:757:ARG:NH1	1:B:780:GLU:OE1	2.52	0.42
1:B:281:VAL:HG11	2:D:3:A:C2	2.54	0.42
1:A:175:ARG:O	1:A:179:THR:OG1	2.35	0.42
1:A:435:MET:O	1:A:439:VAL:HG23	2.19	0.42
1:A:545:ALA:HA	1:A:548:GLU:HG3	2.02	0.42
1:B:176:ALA:O	1:B:180:VAL:HG23	2.20	0.42
1:B:605:ILE:HD12	1:B:605:ILE:HA	1.80	0.42
1:B:775:LEU:O	1:B:778:TYR:N	2.48	0.42
1:B:88:LEU:HD12	1:B:88:LEU:HA	1.86	0.42
1:B:143:MET:HB2	1:B:143:MET:HE2	1.93	0.42
1:B:330:PHE:HD1	1:B:330:PHE:HA	1.74	0.42
1:B:478:TYR:O	1:B:482:THR:HG23	2.18	0.42
1:B:575:ARG:NH1	1:B:608:LYS:HE3	2.34	0.42
1:B:482:THR:OG1	1:B:483:SER:N	2.53	0.41
1:A:647:SER:OG	1:A:676:GLY:O	2.34	0.41
1:A:74:PRO:HG2	1:A:75:ASP:H	1.85	0.41
2:D:9:U:O4'	2:D:9:U:P	2.78	0.41
1:A:296:TYR:HE1	1:A:300:LEU:CD1	2.00	0.41
1:B:248:ALA:O	1:B:252:ILE:HG13	2.20	0.41
1:B:559:PRO:CD	1:B:590:ARG:NH2	2.83	0.41
1:B:637:LEU:HA	1:B:637:LEU:HD23	1.72	0.41
2:D:14:A:O2'	2:D:15:U:P	2.78	0.41
2:D:5:U:HO2'	2:D:6:C:P	2.30	0.41
1:A:267:PHE:O	1:A:271:LEU:HB2	2.21	0.41
1:A:288:GLN:OE1	1:A:292:LYS:HE2	2.20	0.41
1:A:291:GLY:CA	1:A:324:THR:CG2	2.87	0.41
1:A:760:LEU:CD1	1:A:760:LEU:C	2.88	0.41
1:B:551:VAL:CG1	1:B:557:VAL:O	2.64	0.41
1:A:728:MET:O	1:A:732:GLY:N	2.54	0.41
1:B:284:ASN:ND2	1:B:317:THR:HB	2.36	0.41
1:B:535:TYR:CZ	1:B:543:GLY:HA3	2.55	0.41
1:A:775:LEU:HA	1:A:775:LEU:HD12	1.95	0.41
1:B:210:VAL:HG21	2:D:1:G:O6	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:747:TYR:HB3	1:B:756:ALA:HB2	2.03	0.41
1:A:341:MET:O	1:A:341:MET:SD	2.79	0.41
1:A:532:LEU:HD12	1:A:532:LEU:HA	1.87	0.41
1:B:599:PHE:HB3	1:B:622:ILE:CG1	2.50	0.41
1:A:524:ASN:HD22	1:A:524:ASN:N	2.19	0.41
1:B:398:LYS:HA	1:B:398:LYS:HD3	1.58	0.41
1:A:632:ILE:HD13	2:D:14:A:N3	2.36	0.41
1:A:316:VAL:O	1:A:320:GLU:HG3	2.21	0.41
1:A:338:LEU:CD2	1:A:375:GLN:HB2	2.50	0.41
1:A:353:TYR:CD2	1:A:376:MET:HG3	2.56	0.41
1:A:585:GLN:NE2	1:A:586:GLU:OE2	2.53	0.41
1:A:598:ILE:O	1:A:602:MET:HG2	2.20	0.41
1:A:74:PRO:C	1:A:76:ALA:H	2.24	0.41
1:B:191:GLU:O	1:B:195:GLU:HG3	2.20	0.41
1:B:690:LEU:O	1:B:693:MET:HB3	2.20	0.41
1:B:715:LEU:O	1:B:716:GLU:O	2.39	0.41
1:A:586:GLU:HA	1:A:589:ALA:HB3	2.03	0.41
1:B:319:ASN:O	1:B:322:ALA:HB3	2.20	0.41
1:B:495:ALA:O	1:B:498:ASN:HB3	2.21	0.41
1:A:340:THR:C	1:A:342:ALA:N	2.73	0.41
1:B:532:LEU:HD11	1:B:547:ILE:HG21	2.02	0.41
1:B:564:LEU:HB3	1:B:587:VAL:HG22	2.03	0.41
1:B:623:LYS:C	1:B:625:SER:N	2.73	0.41
1:A:141:LEU:HD23	1:A:166:LEU:HD11	2.03	0.40
1:A:737:GLU:N	1:A:737:GLU:OE1	2.54	0.40
1:B:560:SER:OG	1:B:562:VAL:CG2	2.69	0.40
1:A:287:LEU:HD13	1:A:299:ALA:CA	2.52	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:B:223:GLY:O	1:B:225:SER:OG	2.24	0.40
1:B:73:SER:HA	1:B:74:PRO:HD3	1.90	0.40
1:A:660:SER:O	1:A:662:THR:N	2.54	0.40
1:A:761:SER:C	1:A:763:VAL:N	2.74	0.40
1:B:174:VAL:HG11	1:B:208:THR:HG23	2.04	0.40
1:B:79:LEU:O	1:B:83:ILE:HG13	2.22	0.40
1:B:96:ALA:O	1:B:99:ARG:HB2	2.21	0.40
1:A:660:SER:C	1:A:662:THR:N	2.73	0.40
1:B:478:TYR:CD1	1:B:496:LEU:HD11	2.56	0.40
1:A:353:TYR:CE2	1:A:381:PHE:CD2	3.07	0.40
1:A:544:ILE:O	1:A:547:ILE:N	2.45	0.40
1:A:657:LEU:O	1:A:663:MET:O	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:LEU:HD12	1:B:531:LEU:HA	1.92	0.40
1:A:524:ASN:ND2	1:B:590:ARG:O	2.55	0.40
1:B:614:LYS:O	1:B:618:VAL:HG23	2.22	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:168:PRO:O	1:A:447:ARG:NH1[1_565]	1.96	0.24
1:A:413:ARG:NE	1:B:518:THR:O[3_744]	2.16	0.04

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	677/718 (94%)	599 (88%)	65 (10%)	13 (2%)	8	26
1	B	671/718 (94%)	605 (90%)	50 (8%)	16 (2%)	6	20
All	All	1348/1436 (94%)	1204 (89%)	115 (8%)	29 (2%)	6	22

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

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Mol	Chain	Res	Type
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%)	456 (85%)	83 (15%)	2	8
1	B	530/587 (90%)	476 (90%)	54 (10%)	7	22
All	All	1069/1174 (91%)	932 (87%)	137 (13%)	4	13

All (137) 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

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Mol	Chain	Res	Type
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	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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 [i](#)

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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	0.92	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	548:GLU	C	549:ASN	N	1.17

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	687/718 (95%)	0.19	36 (5%) 27 18	32, 75, 135, 243	104 (15%)
1	B	683/718 (95%)	0.26	35 (5%) 28 19	40, 74, 128, 237	86 (12%)
2	C	14/18 (77%)	-0.02	0 100 100	56, 82, 108, 120	4 (28%)
2	D	18/18 (100%)	0.59	1 (5%) 24 16	73, 89, 135, 158	7 (38%)
All	All	1402/1472 (95%)	0.23	72 (5%) 28 19	32, 75, 133, 243	201 (14%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	784	PHE	12.0
1	B	329	GLY	7.9
1	B	780	GLU	6.0
1	B	750	ALA	5.8
1	B	748	CYS	5.8
1	B	752	ARG	5.4
1	B	293	ALA	5.4
1	A	712	TYR	5.2
1	B	327	ARG	5.1
1	B	744	VAL	5.0
1	A	750	ALA	4.7
1	A	713	SER	4.5
1	B	747	TYR	4.5
1	A	761	SER	4.4
1	B	611	MET	4.2
1	B	782	ALA	4.1
1	B	610	GLY	4.0
1	A	324	THR	3.8
1	A	748	CYS	3.7
1	A	774	ALA	3.6
1	A	778	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	744	VAL	3.5
1	A	294	GLY	3.5
1	B	268	PHE	3.5
1	A	379	THR	3.4
2	D	13	U	3.4
1	A	740	TYR	3.4
1	A	116	LEU	3.3
1	A	745	GLU	3.3
1	B	328	ALA	3.2
1	B	776	GLU	3.1
1	B	746	SER	3.0
1	A	746	SER	2.9
1	B	716	GLU	2.9
1	A	341	MET	2.9
1	A	364	GLY	2.9
1	A	747	TYR	2.8
1	A	759	PHE	2.8
1	B	751	LYS	2.8
1	A	293	ALA	2.8
1	A	292	LYS	2.7
1	B	627	LEU	2.7
1	B	593	ASN	2.7
1	B	758	GLY	2.7
1	B	783	GLN	2.6
1	A	775	LEU	2.6
1	B	753	PHE	2.6
1	A	278	PRO	2.6
1	B	779	ILE	2.6
1	B	415	GLY	2.5
1	B	331	PHE	2.5
1	A	163	GLU	2.5
1	A	682	LEU	2.5
1	B	115	GLU	2.5
1	B	100	ASP	2.4
1	B	281	VAL	2.4
1	A	728	MET	2.4
1	A	296	TYR	2.4
1	A	277	ALA	2.3
1	A	378	LYS	2.3
1	B	290	PHE	2.3
1	B	330	PHE	2.3
1	A	708	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	348	PRO	2.2
1	A	365	LYS	2.2
1	B	557	VAL	2.2
1	A	554	SER	2.1
1	A	741	ARG	2.1
1	B	759	PHE	2.1
1	A	640	MET	2.1
1	A	186	ARG	2.1
1	B	641	TYR	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PO4	B	801	5/5	-	-	78,79,79,79	5

6.5 Other polymers [i](#)

There are no such residues in this entry.