



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:04 AM UTC

PDB ID : 1S77 / pdb_00001s77
Title : T7 RNAP product pyrophosphate elongation complex
Authors : Yin, Y.W.; Steitz, T.A.
Deposited on : 2004-01-29
Resolution : 2.69 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

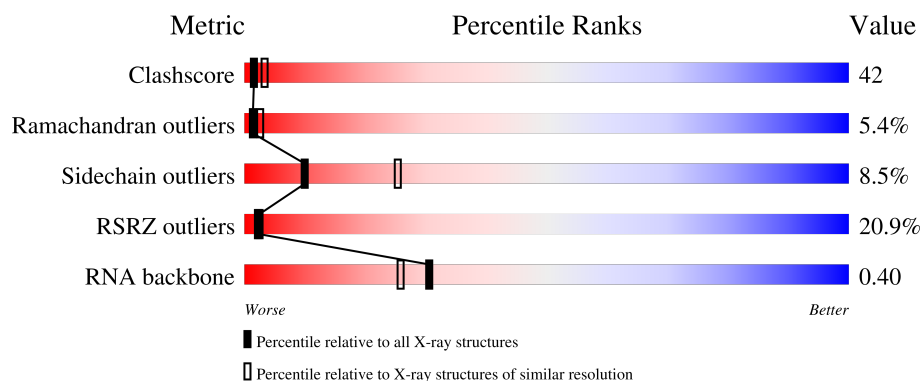
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	T	21	67% 14% 62% 5% 19%
2	N	17	88% 18% 82%
3	R	10	60% 10% 70% 20%
4	D	883	17% 38% 46% 10% 6%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7540 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 DNA chain called DNA (5'-D(*GP*CP*CP*GP*TP*GP*CP*GP*CP*AP*TP*TP*CP*GP*CP*CP*GP*TP*GP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	21	Total	C	N	O	P	0	0	0
			425	203	73	129	20			

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*TP*TP*AP*CP*GP*TP*TP*GP*CP*GP*CP*AP*CP*GP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	17	Total	C	N	O	P	0	0	0
			344	165	60	103	16			

- Molecule 3 is a RNA chain called RNA (5'-R(*AP*CP*AP*CP*GP*GP*CP*GP*AP*(3D A))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	10	Total	C	N	O	P	0	0	0
			213	97	44	63	9			

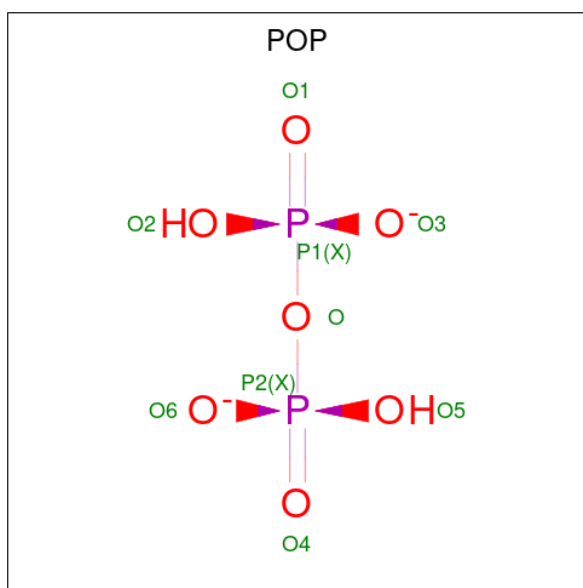
- Molecule 4 is a protein called DNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	828	Total	C	N	O	S	0	0	0
			6546	4177	1139	1195	35			

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	R	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

- Molecule 6 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	O	P	0	0
			9	7	2		

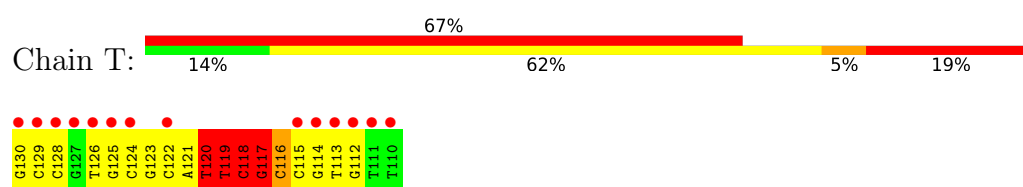
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	O	0	0
			1	1		

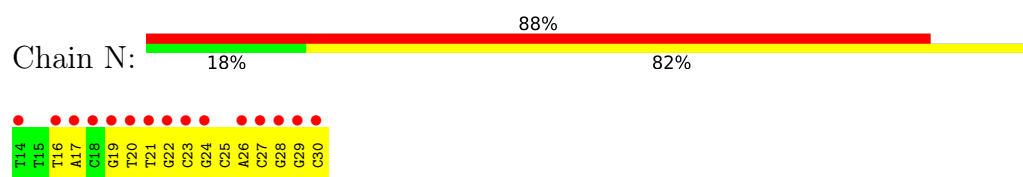
3 Residue-property plots

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

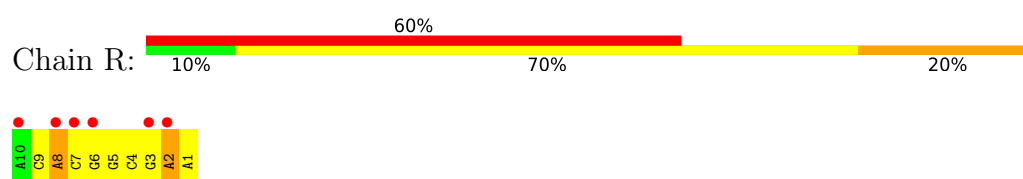
- Molecule 1: DNA (5'-D(*GP*CP*CP*GP*TP*GP*CP*GP*CP*AP*TP*TP*CP*GP*CP*CP*GP*TP*GP*TP*T)-3')



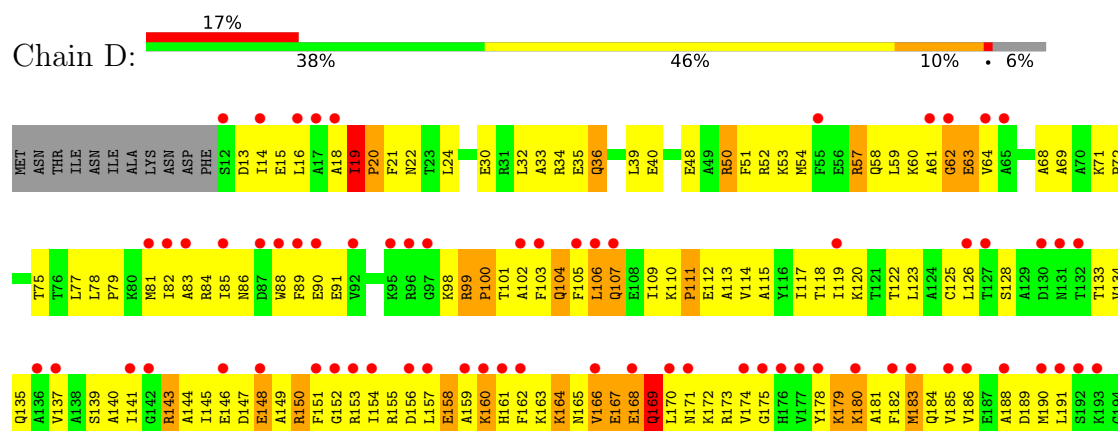
- Molecule 2: DNA (5'-D(*TP*TP*TP*AP*CP*GP*TP*TP*GP*CP*GP*CP*AP*CP*GP*GP*C)-3')

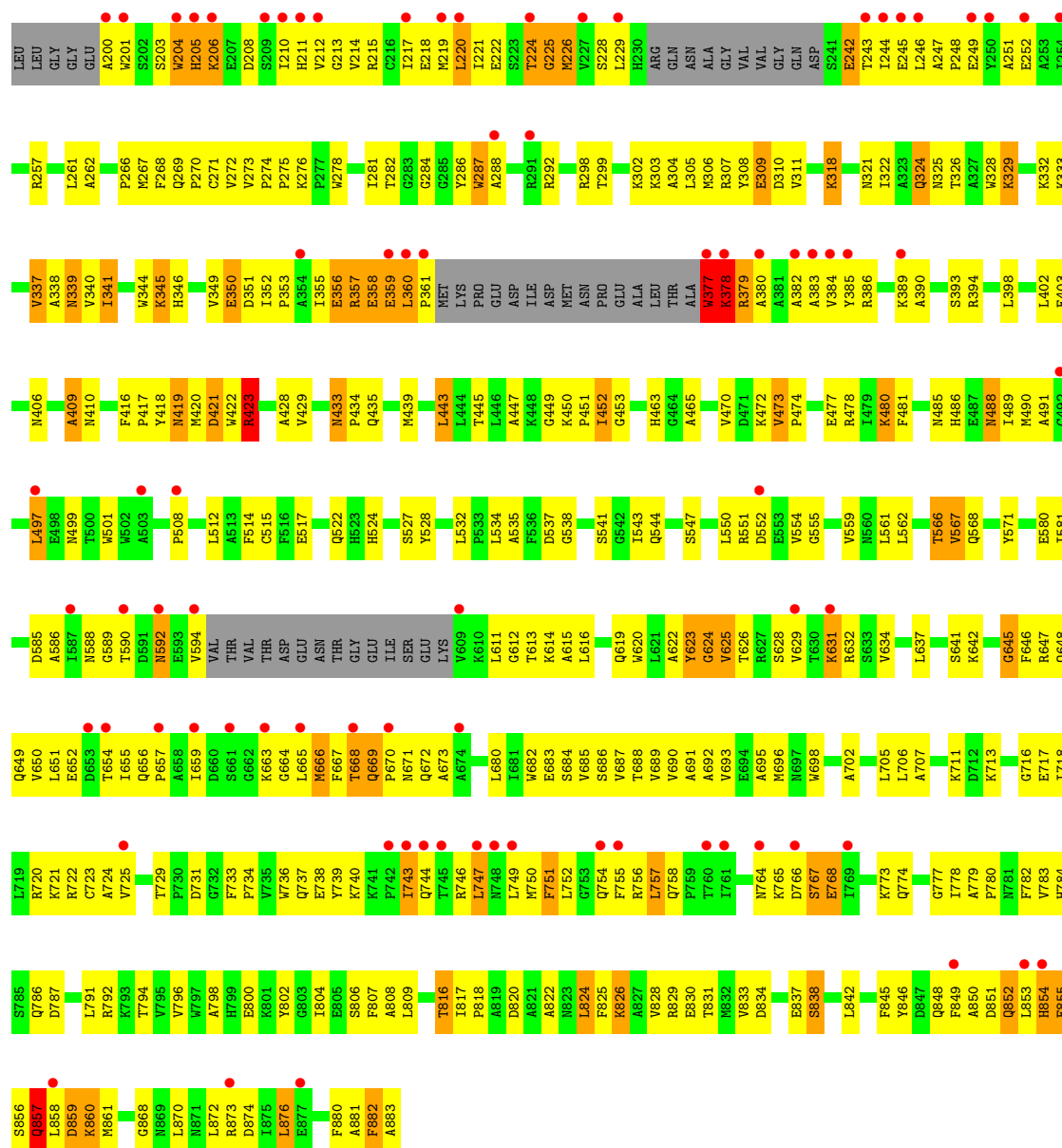


- Molecule 3: RNA (5'-R(*AP*CP*AP*CP*GP*GP*CP*GP*AP*(3DA))-3')



- Molecule 4: DNA-directed RNA polymerase





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	127.74Å 141.84Å 142.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.69 30.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-2.69) 92.3 (30.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.72Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.251 , 0.285 0.253 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	53.3	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7540	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 3DA, POP

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	T	0.32	0/474	0.94	6/730 (0.8%)
2	N	0.25	0/384	0.57	0/591
3	R	0.30	0/215	0.57	0/334
4	D	0.54	2/6698 (0.0%)	1.05	37/9060 (0.4%)
All	All	0.51	2/7771 (0.0%)	1.01	43/10715 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	T	0	5
4	D	0	2
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	180	LYS	C-N	9.12	1.46	1.33
4	D	377	TRP	C-N	-8.84	1.21	1.33

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	378	LYS	CA-C-N	-19.88	83.57	121.54
4	D	378	LYS	C-N-CA	-19.88	83.57	121.54
4	D	378	LYS	O-C-N	14.71	142.15	122.59
4	D	377	TRP	CA-C-N	9.51	139.69	121.54
4	D	377	TRP	C-N-CA	9.51	139.69	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	860	LYS	N-CA-C	-9.32	101.22	112.59
4	D	377	TRP	O-C-N	-8.45	109.48	123.00
4	D	179	LYS	CA-C-N	-8.06	108.90	122.11
4	D	179	LYS	C-N-CA	-8.06	108.90	122.11
1	T	117	DG	N9-C1'-C2'	-7.36	102.47	113.50
4	D	535	ALA	N-CA-C	7.29	121.34	109.76
4	D	837	GLU	N-CA-C	-7.16	104.69	113.50
1	T	119	DT	C5'-C4'-C3'	-6.92	104.52	114.90
4	D	220	LEU	N-CA-C	-6.91	103.50	112.68
4	D	19	ILE	CA-C-N	6.89	128.45	119.84
4	D	19	ILE	C-N-CA	6.89	128.45	119.84
4	D	808	ALA	N-CA-C	-6.63	96.41	108.02
4	D	380	ALA	N-CA-C	-6.56	105.03	113.16
4	D	880	PHE	N-CA-C	6.45	121.30	113.17
4	D	428	ALA	N-CA-C	-6.38	101.50	110.50
4	D	287	TRP	N-CA-C	6.32	119.46	111.69
4	D	409	ALA	N-CA-C	-6.30	102.66	110.41
1	T	117	DG	C4'-C3'-O3'	6.17	119.26	110.00
1	T	118	DC	C5'-C4'-C3'	-6.13	105.71	114.90
4	D	824	LEU	N-CA-C	-6.11	104.68	111.71
4	D	99	ARG	CA-C-N	5.90	127.21	119.84
4	D	99	ARG	C-N-CA	5.90	127.21	119.84
4	D	148	GLU	N-CA-C	-5.88	105.00	111.82
4	D	423	ARG	N-CA-C	-5.86	106.13	113.28
4	D	580	GLU	N-CA-C	-5.84	104.82	111.07
4	D	421	ASP	N-CA-C	-5.82	103.02	110.53
4	D	205	HIS	CB-CA-C	-5.72	110.00	116.63
4	D	394	ARG	N-CA-C	-5.54	105.39	111.82
4	D	345	LYS	N-CA-C	-5.46	104.36	111.02
1	T	117	DG	C5'-C4'-C3'	-5.42	106.76	114.90
4	D	389	LYS	N-CA-C	-5.30	105.40	111.07
4	D	422	TRP	N-CA-C	5.29	119.21	112.87
4	D	169	GLN	N-CA-C	-5.19	104.49	111.54
4	D	524	HIS	N-CA-C	5.17	121.31	114.12
4	D	645	GLY	N-CA-C	-5.16	106.25	112.49
4	D	166	VAL	N-CA-C	-5.12	106.10	113.07
1	T	120	DT	C5'-C4'-C3'	-5.10	107.24	114.90
4	D	452	ILE	N-CA-C	5.05	115.27	110.42

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	377	TRP	Peptide
4	D	378	LYS	Mainchain
1	T	116	DC	Sidechain
1	T	117	DG	Sidechain
1	T	118	DC	Sidechain
1	T	119	DT	Sidechain
1	T	120	DT	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	425	0	239	29	0
2	N	344	0	194	25	0
3	R	213	0	112	19	0
4	D	6546	0	6518	574	0
5	D	1	0	0	0	0
5	R	1	0	0	0	0
6	D	9	0	0	0	0
7	D	1	0	0	1	0
All	All	7540	0	7063	619	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 42.

All (619) 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)
4:D:377:TRP:O	4:D:379:ARG:N	1.61	1.32
4:D:147:ASP:OD1	4:D:180:LYS:NZ	1.77	1.15
4:D:378:LYS:O	4:D:379:ARG:O	1.75	1.04
4:D:298:ARG:NH2	4:D:419:ASN:HD21	1.55	1.03
4:D:164:LYS:HB3	4:D:166:VAL:HG23	1.40	1.02
4:D:702:ALA:HA	4:D:861:MET:HE1	1.38	1.00
4:D:433:ASN:HD22	4:D:435:GLN:H	1.05	0.99
2:N:17:DA:OP2	4:D:378:LYS:HE3	1.62	0.98
4:D:298:ARG:HH21	4:D:419:ASN:ND2	1.63	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:873:ARG:HH11	4:D:873:ARG:HB2	1.30	0.95
4:D:856:SER:O	4:D:857:GLN:HB3	1.66	0.95
3:R:9:C:H2'	3:R:8:A:H5''	1.48	0.95
4:D:613:THR:HG22	4:D:614:LYS:H	1.32	0.94
4:D:278:TRP:H	4:D:321:ASN:HD21	0.95	0.94
2:N:16:DT:H4'	4:D:378:LYS:HD3	1.51	0.93
4:D:298:ARG:HH21	4:D:419:ASN:HD21	0.99	0.93
4:D:133:THR:HG22	4:D:243:THR:HG22	1.48	0.92
4:D:739:TYR:H	4:D:774:GLN:NE2	1.70	0.89
4:D:581:ILE:HG21	4:D:680:LEU:HD22	1.53	0.89
4:D:281:ILE:HG13	4:D:282:THR:HG23	1.54	0.89
4:D:340:VAL:HG23	4:D:341:ILE:H	1.37	0.88
4:D:175:GLY:HA3	4:D:178:TYR:HB2	1.53	0.88
4:D:215:ARG:HG3	4:D:219:MET:HE3	1.55	0.87
4:D:167:GLU:HB2	4:D:170:LEU:HA	1.56	0.87
4:D:173:ARG:H	4:D:173:ARG:HD3	1.43	0.83
4:D:592:ASN:HD22	4:D:592:ASN:N	1.74	0.83
4:D:473:VAL:HG21	4:D:477:GLU:OE1	1.80	0.82
4:D:378:LYS:C	4:D:379:ARG:O	2.20	0.81
4:D:873:ARG:HB2	4:D:873:ARG:NH1	1.95	0.81
4:D:798:ALA:HB1	4:D:804:ILE:HD12	1.60	0.81
4:D:278:TRP:H	4:D:321:ASN:ND2	1.77	0.80
3:R:9:C:C2'	3:R:8:A:H5''	2.13	0.79
1:T:112:DG:H2'	4:D:57:ARG:HH22	1.48	0.78
4:D:377:TRP:O	4:D:379:ARG:CA	2.32	0.78
4:D:377:TRP:O	4:D:379:ARG:CB	2.32	0.77
4:D:210:ILE:O	4:D:214:VAL:HG23	1.85	0.77
4:D:816:THR:OG1	4:D:824:LEU:HD22	1.85	0.77
4:D:78:LEU:HB3	4:D:79:PRO:HD3	1.66	0.77
4:D:473:VAL:HG22	4:D:474:PRO:HD2	1.66	0.77
4:D:739:TYR:H	4:D:774:GLN:HE21	1.30	0.76
4:D:829:ARG:NH2	4:D:882:PHE:H	1.83	0.76
1:T:116:DC:H2''	1:T:115:DC:OP2	1.83	0.76
4:D:139:SER:O	4:D:143:ARG:HB2	1.86	0.76
2:N:16:DT:C4'	4:D:378:LYS:HD3	2.15	0.76
4:D:713:LYS:H	4:D:713:LYS:HD2	1.50	0.75
4:D:183:MET:HE2	4:D:186:VAL:HG21	1.69	0.75
4:D:340:VAL:HG23	4:D:341:ILE:N	2.02	0.74
4:D:834:ASP:O	4:D:838:SER:HB2	1.87	0.74
4:D:215:ARG:O	4:D:219:MET:HG2	1.88	0.73
4:D:275:PRO:HB2	4:D:324:GLN:HG3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:119:DT:H2''	1:T:118:DC:OP2	1.85	0.73
4:D:298:ARG:CZ	4:D:419:ASN:HD21	2.01	0.73
4:D:791:LEU:HD21	4:D:809:LEU:HD13	1.71	0.72
4:D:826:LYS:O	4:D:830:GLU:HG3	1.90	0.72
4:D:796:VAL:O	4:D:800:GLU:HG3	1.90	0.72
4:D:303:LYS:HE2	4:D:303:LYS:H	1.55	0.71
4:D:180:LYS:O	4:D:184:GLN:HB3	1.91	0.71
2:N:27:DC:H2''	2:N:28:DG:O5'	1.89	0.71
4:D:551:ARG:HG3	4:D:551:ARG:HH11	1.53	0.71
4:D:54:MET:O	4:D:57:ARG:HG3	1.91	0.70
4:D:249:GLU:CD	4:D:249:GLU:H	1.99	0.70
4:D:450:LYS:HG3	4:D:817:ILE:CD1	2.20	0.70
4:D:853:LEU:O	4:D:854:HIS:HB2	1.90	0.70
4:D:53:LYS:HD3	4:D:54:MET:N	2.06	0.70
4:D:497:LEU:HD12	4:D:497:LEU:H	1.57	0.70
4:D:746:ARG:HD2	4:D:754:GLN:CD	2.17	0.70
4:D:180:LYS:O	4:D:180:LYS:HG3	1.91	0.70
4:D:36:GLN:HE21	4:D:272:VAL:H	1.40	0.69
4:D:117:ILE:HG12	4:D:752:LEU:HD22	1.75	0.69
4:D:201:TRP:HZ2	4:D:204:TRP:HE1	1.41	0.69
4:D:740:LYS:HD3	4:D:767:SER:HB3	1.75	0.69
4:D:79:PRO:O	4:D:82:ILE:HG22	1.93	0.69
4:D:747:LEU:HD23	4:D:747:LEU:H	1.58	0.68
4:D:228:SER:C	4:D:229:LEU:HD22	2.18	0.68
4:D:119:ILE:HG23	4:D:226:MET:HE1	1.74	0.68
4:D:286:TYR:CZ	4:D:417:PRO:HG3	2.29	0.68
4:D:592:ASN:N	4:D:592:ASN:ND2	2.42	0.68
3:R:4:C:H2'	3:R:3:G:C8	2.27	0.67
4:D:472:LYS:C	4:D:567:VAL:HG11	2.19	0.67
4:D:550:LEU:HD11	4:D:695:ALA:HB2	1.76	0.67
4:D:13:ASP:HB3	4:D:16:LEU:HD13	1.76	0.67
4:D:13:ASP:HB3	4:D:16:LEU:HD22	1.74	0.67
4:D:816:THR:HG22	4:D:817:ILE:H	1.59	0.67
4:D:421:ASP:OD1	4:D:423:ARG:NH1	2.28	0.67
4:D:589:GLY:O	4:D:613:THR:HB	1.94	0.67
4:D:244:ILE:HD12	4:D:244:ILE:O	1.95	0.67
4:D:35:GLU:HG2	4:D:272:VAL:HG21	1.77	0.66
4:D:433:ASN:ND2	4:D:435:GLN:H	1.86	0.66
4:D:104:GLN:NE2	4:D:104:GLN:H	1.92	0.66
4:D:806:SER:O	4:D:816:THR:HG23	1.96	0.66
4:D:82:ILE:C	4:D:84:ARG:H	2.03	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:586:ALA:O	4:D:614:LYS:HG3	1.95	0.66
2:N:25:DC:H1'	2:N:26:DA:H5''	1.77	0.66
4:D:551:ARG:HE	4:D:872:LEU:HD11	1.59	0.66
4:D:146:GLU:O	4:D:148:GLU:N	2.29	0.66
4:D:148:GLU:O	4:D:152:GLY:HA3	1.96	0.66
4:D:378:LYS:O	4:D:382:ALA:CB	2.43	0.65
3:R:3:G:H2'	3:R:2:A:O4'	1.95	0.65
4:D:647:ARG:HH21	4:D:671:ASN:ND2	1.95	0.65
4:D:82:ILE:HB	4:D:112:GLU:CD	2.22	0.65
4:D:123:LEU:C	4:D:125:CYS:H	2.05	0.65
4:D:378:LYS:O	4:D:382:ALA:HB2	1.97	0.64
4:D:89:PHE:C	4:D:91:GLU:H	2.06	0.64
3:R:9:C:H2'	3:R:8:A:C5'	2.26	0.64
4:D:59:LEU:HB3	4:D:64:VAL:HG22	1.79	0.64
4:D:833:VAL:HG21	4:D:876:LEU:HD13	1.77	0.64
4:D:329:LYS:HG2	4:D:447:ALA:HA	1.80	0.64
4:D:690:VAL:HG23	4:D:691:ALA:N	2.12	0.64
4:D:383:ALA:O	4:D:386:ARG:HB3	1.97	0.64
4:D:767:SER:O	4:D:768:GLU:HB3	1.97	0.64
1:T:120:DT:H2''	1:T:119:DT:OP2	1.98	0.64
1:T:118:DC:H2''	1:T:117:DG:OP2	1.96	0.63
4:D:181:ALA:O	4:D:184:GLN:HG2	1.98	0.63
4:D:723:CYS:HB3	4:D:853:LEU:HD13	1.80	0.63
4:D:68:ALA:HB3	4:D:261:LEU:HD21	1.80	0.63
4:D:613:THR:HG22	4:D:614:LYS:N	2.08	0.63
2:N:17:DA:P	4:D:378:LYS:HE3	2.37	0.63
4:D:409:ALA:O	4:D:410:ASN:HB2	1.97	0.63
4:D:117:ILE:HG23	4:D:752:LEU:HD21	1.80	0.63
4:D:707:ALA:O	4:D:722:ARG:HG2	1.99	0.63
4:D:766:ASP:O	4:D:767:SER:HB2	1.96	0.63
4:D:278:TRP:N	4:D:321:ASN:HD21	1.81	0.63
4:D:339:ASN:HD21	4:D:406:ASN:HD21	1.46	0.63
4:D:148:GLU:OE1	4:D:749:LEU:HB3	1.98	0.63
4:D:257:ARG:O	4:D:261:LEU:HB2	1.99	0.63
4:D:302:LYS:NZ	4:D:302:LYS:HB3	2.14	0.63
4:D:57:ARG:HD3	4:D:57:ARG:C	2.24	0.62
4:D:69:ALA:HA	4:D:257:ARG:CG	2.28	0.62
4:D:133:THR:HB	4:D:242:GLU:O	1.99	0.62
4:D:358:GLU:N	4:D:358:GLU:CD	2.58	0.62
4:D:551:ARG:HE	4:D:872:LEU:CD1	2.13	0.62
4:D:205:HIS:C	4:D:206:LYS:HE3	2.24	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:702:ALA:CA	4:D:861:MET:HE1	2.23	0.62
4:D:159:ALA:C	4:D:161:HIS:H	2.07	0.62
4:D:299:THR:HB	4:D:304:ALA:HB3	1.82	0.61
4:D:377:TRP:O	4:D:379:ARG:HB3	2.00	0.61
4:D:84:ARG:HA	4:D:84:ARG:NE	2.16	0.61
4:D:611:LEU:HD13	4:D:619:GLN:HE22	1.64	0.61
4:D:855:GLU:CD	4:D:856:SER:N	2.58	0.61
3:R:9:C:C3'	3:R:8:A:H5''	2.29	0.61
4:D:750:MET:O	4:D:751:PHE:HB2	2.01	0.61
4:D:154:ILE:HD11	4:D:158:GLU:HG2	1.82	0.61
4:D:81:MET:HG3	4:D:115:ALA:HB1	1.81	0.61
4:D:84:ARG:HD3	4:D:222:GLU:HG2	1.83	0.61
3:R:9:C:H5'	4:D:746:ARG:HH21	1.64	0.61
4:D:345:LYS:HD2	4:D:346:HIS:CE1	2.35	0.60
4:D:141:ILE:O	4:D:145:ILE:HG12	2.01	0.60
4:D:624:GLY:O	4:D:626:THR:HG23	2.01	0.60
4:D:784:HIS:HA	4:D:787:ASP:OD2	2.01	0.60
4:D:433:ASN:HD22	4:D:435:GLN:N	1.89	0.60
4:D:828:VAL:HG21	4:D:883:ALA:HA	1.84	0.60
4:D:713:LYS:HD2	4:D:713:LYS:N	2.16	0.60
4:D:845:PHE:O	4:D:848:GLN:HB2	2.01	0.60
4:D:480:LYS:HE2	4:D:480:LYS:HA	1.84	0.60
4:D:720:ARG:HH12	4:D:858:LEU:CD1	2.15	0.60
4:D:723:CYS:SG	4:D:853:LEU:HB3	2.41	0.60
4:D:851:ASP:CG	4:D:852:GLN:H	2.09	0.59
4:D:275:PRO:CB	4:D:324:GLN:HG3	2.32	0.59
4:D:164:LYS:HB3	4:D:166:VAL:CG2	2.25	0.59
4:D:852:GLN:HG2	4:D:853:LEU:HG	1.82	0.59
4:D:747:LEU:HD23	4:D:747:LEU:N	2.17	0.59
4:D:137:VAL:CG2	4:D:244:ILE:HG12	2.33	0.59
4:D:160:LYS:HB2	4:D:160:LYS:NZ	2.17	0.59
4:D:163:LYS:C	4:D:165:ASN:H	2.10	0.59
4:D:206:LYS:HE3	4:D:206:LYS:N	2.17	0.59
4:D:846:TYR:HA	4:D:849:PHE:CE1	2.38	0.59
4:D:101:THR:HA	4:D:104:GLN:OE1	2.02	0.59
4:D:204:TRP:CZ3	4:D:212:VAL:HG21	2.36	0.59
4:D:120:LYS:O	4:D:120:LYS:HD3	2.03	0.59
4:D:182:PHE:O	4:D:183:MET:HG2	2.03	0.59
4:D:21:PHE:HZ	4:D:30:GLU:HG3	1.68	0.59
4:D:126:LEU:HD13	4:D:246:LEU:HB2	1.85	0.59
4:D:204:TRP:HZ3	4:D:212:VAL:HG21	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:488:ASN:HB3	4:D:501:TRP:CE3	2.38	0.58
4:D:651:LEU:CD1	4:D:670:PRO:HB2	2.33	0.58
4:D:723:CYS:SG	4:D:853:LEU:HD22	2.43	0.58
4:D:133:THR:CG2	4:D:243:THR:HG22	2.29	0.58
4:D:711:LYS:HA	4:D:717:GLU:O	2.02	0.58
4:D:77:LEU:HD13	4:D:224:THR:HB	1.85	0.58
4:D:752:LEU:H	4:D:752:LEU:HD12	1.68	0.58
4:D:229:LEU:HD12	4:D:242:GLU:OE1	2.02	0.58
4:D:585:ASP:HB3	4:D:613:THR:HG22	1.86	0.58
4:D:21:PHE:CZ	4:D:30:GLU:HG3	2.39	0.58
4:D:551:ARG:HG3	4:D:551:ARG:NH1	2.19	0.58
4:D:794:THR:HA	4:D:831:THR:HG21	1.85	0.57
4:D:122:THR:HG22	4:D:141:ILE:HD11	1.86	0.57
4:D:162:PHE:C	4:D:164:LYS:H	2.12	0.57
4:D:214:VAL:HG12	4:D:218:GLU:OE1	2.05	0.57
4:D:417:PRO:HG2	4:D:429:VAL:HB	1.85	0.57
4:D:247:ALA:HB1	4:D:249:GLU:OE2	2.04	0.57
4:D:329:LYS:HG3	4:D:445:THR:HG23	1.86	0.57
4:D:552:ASP:OD2	4:D:552:ASP:C	2.46	0.57
4:D:104:GLN:H	4:D:104:GLN:HE21	1.50	0.57
4:D:541:SER:HA	4:D:544:GLN:HG3	1.86	0.57
4:D:757:LEU:HD23	4:D:758:GLN:N	2.20	0.57
4:D:720:ARG:HG3	4:D:720:ARG:HH11	1.68	0.57
1:T:122:DC:H2''	1:T:121:DA:OP2	2.04	0.56
2:N:27:DC:H2''	2:N:28:DG:H2'	1.86	0.56
4:D:36:GLN:NE2	4:D:272:VAL:H	2.03	0.56
4:D:217:ILE:O	4:D:221:ILE:HG13	2.05	0.56
4:D:705:LEU:HB3	4:D:858:LEU:HD22	1.86	0.56
4:D:53:LYS:HD3	4:D:53:LYS:C	2.31	0.56
4:D:62:GLY:O	4:D:63:GLU:HG3	2.05	0.56
4:D:585:ASP:CG	4:D:613:THR:HG21	2.30	0.56
1:T:119:DT:H5''	4:D:777:GLY:HA2	1.88	0.56
4:D:59:LEU:C	4:D:61:ALA:H	2.10	0.56
4:D:711:LYS:HG2	4:D:718:ILE:HD13	1.87	0.56
4:D:298:ARG:NE	4:D:419:ASN:HD21	2.03	0.56
4:D:161:HIS:O	4:D:164:LYS:HB2	2.06	0.56
3:R:3:G:H3'	3:R:2:A:H5''	1.88	0.56
4:D:71:LYS:N	4:D:72:PRO:HD2	2.21	0.56
4:D:203:SER:C	4:D:205:HIS:H	2.14	0.56
4:D:69:ALA:HA	4:D:257:ARG:HG3	1.87	0.56
4:D:50:ARG:HB3	4:D:267:MET:HE3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:124:DC:H1'	1:T:123:DG:H5'	1.88	0.55
1:T:126:DT:H1'	1:T:125:DG:H5''	1.88	0.55
4:D:452:ILE:HG13	4:D:818:PRO:HB2	1.86	0.55
4:D:671:ASN:O	4:D:673:ALA:N	2.37	0.55
4:D:306:MET:O	4:D:309:GLU:HB3	2.06	0.55
4:D:302:LYS:HB3	4:D:302:LYS:HZ2	1.69	0.55
4:D:684:SER:O	4:D:687:VAL:HG22	2.07	0.55
4:D:48:GLU:HG3	4:D:262:ALA:HB1	1.89	0.55
4:D:137:VAL:HG21	4:D:244:ILE:HG12	1.89	0.55
1:T:112:DG:H2'	4:D:57:ARG:NH2	2.21	0.55
4:D:473:VAL:HG21	4:D:477:GLU:CD	2.32	0.55
1:T:115:DC:C2	3:R:5:G:N2	2.75	0.55
3:R:7:C:H5'	4:D:172:LYS:HE3	1.89	0.55
4:D:19:ILE:HD13	4:D:22:ASN:OD1	2.06	0.55
4:D:85:ILE:O	4:D:88:TRP:HB3	2.07	0.55
4:D:724:ALA:HB1	4:D:738:GLU:HB3	1.89	0.55
3:R:9:C:H1'	4:D:754:GLN:OE1	2.07	0.55
4:D:298:ARG:HE	4:D:419:ASN:ND2	2.05	0.55
4:D:68:ALA:CB	4:D:261:LEU:HD21	2.37	0.54
4:D:738:GLU:HA	4:D:774:GLN:NE2	2.22	0.54
4:D:743:ILE:CD1	4:D:744:GLN:H	2.20	0.54
4:D:612:GLY:O	4:D:616:LEU:HB2	2.07	0.54
4:D:765:LYS:HG2	4:D:766:ASP:OD2	2.08	0.54
2:N:16:DT:H4'	4:D:378:LYS:CD	2.34	0.54
4:D:210:ILE:HG13	4:D:211:HIS:ND1	2.23	0.54
2:N:16:DT:H2''	2:N:17:DA:H5''	1.88	0.54
4:D:145:ILE:O	4:D:149:ALA:HB2	2.08	0.54
4:D:118:THR:HG21	4:D:220:LEU:HD13	1.88	0.54
4:D:326:THR:HG23	4:D:806:SER:HA	1.90	0.54
2:N:24:DG:H2''	2:N:25:DC:C6	2.43	0.54
4:D:170:LEU:N	4:D:170:LEU:HD22	2.23	0.54
4:D:266:PRO:HG2	4:D:268:PHE:CZ	2.43	0.54
4:D:713:LYS:H	4:D:713:LYS:CD	2.18	0.54
4:D:802:TYR:CE1	4:D:826:LYS:HD2	2.43	0.54
4:D:378:LYS:O	4:D:379:ARG:C	2.32	0.53
4:D:538:GLY:HA3	4:D:883:ALA:HB3	1.90	0.53
1:T:114:DG:H2''	1:T:113:DT:OP2	2.08	0.53
4:D:184:GLN:HG3	4:D:185:VAL:HG23	1.89	0.53
4:D:668:THR:O	4:D:669:GLN:HB3	2.08	0.53
4:D:750:MET:SD	4:D:750:MET:N	2.81	0.53
4:D:855:GLU:CD	4:D:857:GLN:H	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:213:GLY:O	4:D:217:ILE:HG13	2.09	0.53
4:D:731:ASP:OD1	4:D:792:ARG:NE	2.42	0.53
1:T:120:DT:H71	4:D:632:ARG:NH2	2.23	0.53
4:D:50:ARG:HG3	4:D:51:PHE:N	2.21	0.53
4:D:184:GLN:HG3	4:D:185:VAL:N	2.24	0.53
4:D:690:VAL:CG2	4:D:691:ALA:N	2.71	0.53
4:D:378:LYS:HA	4:D:382:ALA:HB2	1.90	0.53
4:D:642:LYS:HA	4:D:682:TRP:HZ3	1.74	0.53
1:T:113:DT:H2''	1:T:112:DG:H5'	1.90	0.53
4:D:724:ALA:CB	4:D:738:GLU:HB3	2.39	0.53
2:N:17:DA:H2''	4:D:173:ARG:NH2	2.24	0.53
4:D:537:ASP:O	4:D:882:PHE:HD1	1.92	0.52
4:D:543:ILE:HB	4:D:559:VAL:HG11	1.89	0.52
4:D:105:PHE:O	4:D:106:LEU:HG	2.09	0.52
2:N:20:DT:N3	4:D:647:ARG:NH1	2.55	0.52
4:D:275:PRO:CG	4:D:324:GLN:HG3	2.38	0.52
4:D:634:VAL:HA	4:D:685:VAL:HG21	1.91	0.52
4:D:69:ALA:HA	4:D:257:ARG:HG2	1.91	0.52
2:N:27:DC:C2'	2:N:28:DG:O5'	2.58	0.52
4:D:52:ARG:O	4:D:53:LYS:C	2.53	0.52
4:D:106:LEU:HD23	4:D:145:ILE:HG21	1.92	0.52
4:D:181:ALA:C	4:D:183:MET:H	2.17	0.52
4:D:439:MET:O	4:D:443:LEU:HD22	2.09	0.52
4:D:340:VAL:CG2	4:D:341:ILE:H	2.16	0.52
4:D:656:GLN:N	4:D:657:PRO:HD2	2.25	0.52
4:D:105:PHE:HB3	4:D:212:VAL:HG22	1.91	0.52
4:D:143:ARG:HG3	4:D:143:ARG:HH11	1.75	0.52
2:N:20:DT:H1'	2:N:21:DT:H5'	1.91	0.52
4:D:275:PRO:HG2	4:D:324:GLN:HG3	1.92	0.52
4:D:744:GLN:HB2	4:D:756:ARG:HB3	1.92	0.52
4:D:146:GLU:HA	4:D:149:ALA:HB3	1.92	0.51
1:T:114:DG:H1'	1:T:113:DT:H5'	1.91	0.51
2:N:17:DA:H2''	4:D:173:ARG:CZ	2.40	0.51
4:D:208:ASP:O	4:D:212:VAL:HG23	2.10	0.51
4:D:650:VAL:HG13	4:D:651:LEU:N	2.25	0.51
4:D:150:ARG:HG2	4:D:201:TRP:CE2	2.46	0.51
4:D:828:VAL:CG1	4:D:882:PHE:O	2.59	0.51
4:D:150:ARG:HG2	4:D:201:TRP:CZ2	2.46	0.51
3:R:4:C:H2'	3:R:3:G:H8	1.70	0.51
4:D:84:ARG:O	4:D:88:TRP:HB2	2.10	0.51
2:N:28:DG:H1'	2:N:29:DG:N7	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:59:LEU:HD12	4:D:60:LYS:N	2.26	0.51
4:D:146:GLU:OE1	4:D:204:TRP:HB2	2.09	0.51
4:D:585:ASP:O	4:D:614:LYS:HA	2.11	0.51
4:D:873:ARG:HH11	4:D:873:ARG:CB	2.14	0.51
4:D:386:ARG:HH11	4:D:386:ARG:HG2	1.75	0.51
4:D:123:LEU:C	4:D:125:CYS:N	2.70	0.50
4:D:159:ALA:C	4:D:161:HIS:N	2.70	0.50
4:D:120:LYS:NZ	4:D:752:LEU:O	2.44	0.50
4:D:450:LYS:HG3	4:D:817:ILE:HD11	1.94	0.50
4:D:109:ILE:HD11	4:D:145:ILE:HG23	1.92	0.50
4:D:110:LYS:HB2	4:D:113:ALA:CB	2.41	0.50
4:D:201:TRP:HZ2	4:D:204:TRP:NE1	2.08	0.50
4:D:210:ILE:HG13	4:D:211:HIS:H	1.77	0.50
4:D:648:GLN:HE22	4:D:652:GLU:HB2	1.77	0.50
4:D:40:GLU:CD	4:D:286:TYR:HB3	2.36	0.50
4:D:613:THR:O	4:D:615:ALA:N	2.45	0.50
4:D:450:LYS:HG3	4:D:817:ILE:HD12	1.92	0.50
4:D:744:GLN:HB3	4:D:757:LEU:H	1.77	0.50
4:D:140:ALA:O	4:D:144:ALA:N	2.42	0.49
4:D:190:MET:HG3	4:D:191:LEU:N	2.27	0.49
4:D:377:TRP:C	4:D:379:ARG:CB	2.83	0.49
4:D:246:LEU:HG	4:D:251:ALA:HB2	1.94	0.49
4:D:620:TRP:CZ2	4:D:655:ILE:HD11	2.47	0.49
4:D:693:VAL:HG13	4:D:696:MET:CE	2.42	0.49
4:D:82:ILE:C	4:D:84:ARG:N	2.70	0.49
2:N:19:DG:H1'	2:N:20:DT:H71	1.93	0.49
4:D:629:VAL:HA	4:D:654:THR:HG21	1.94	0.49
4:D:155:ARG:HD3	4:D:155:ARG:C	2.37	0.49
4:D:378:LYS:O	4:D:382:ALA:HB3	2.12	0.49
4:D:489:ILE:HG23	4:D:515:CYS:SG	2.53	0.49
4:D:743:ILE:HD12	4:D:744:GLN:H	1.78	0.49
4:D:30:GLU:CD	4:D:34:ARG:HH21	2.20	0.49
4:D:71:LYS:HD2	4:D:71:LYS:O	2.13	0.49
4:D:669:GLN:NE2	4:D:672:GLN:HE21	2.10	0.49
4:D:337:VAL:HG21	4:D:512:LEU:CD2	2.43	0.49
4:D:552:ASP:OD2	4:D:554:VAL:N	2.46	0.49
4:D:175:GLY:HA3	4:D:178:TYR:CB	2.35	0.49
4:D:298:ARG:HE	4:D:419:ASN:CG	2.21	0.48
4:D:332:LYS:HE3	4:D:410:ASN:H	1.77	0.48
4:D:210:ILE:HG13	4:D:211:HIS:N	2.28	0.48
4:D:318:LYS:O	4:D:322:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:353:PRO:HG2	4:D:398:LEU:HD13	1.95	0.48
4:D:705:LEU:HD22	4:D:858:LEU:HD22	1.95	0.48
4:D:82:ILE:HG13	4:D:86:ASN:CG	2.38	0.48
1:T:112:DG:C2'	4:D:57:ARG:HH22	2.24	0.48
4:D:378:LYS:O	4:D:378:LYS:HD2	2.13	0.48
4:D:846:TYR:CE1	4:D:850:ALA:HB2	2.48	0.48
4:D:167:GLU:CB	4:D:170:LEU:HA	2.37	0.48
4:D:54:MET:O	4:D:58:GLN:HG2	2.13	0.48
4:D:77:LEU:O	4:D:78:LEU:C	2.55	0.48
4:D:98:LYS:HD2	4:D:99:ARG:H	1.79	0.48
4:D:163:LYS:C	4:D:165:ASN:N	2.72	0.48
4:D:214:VAL:O	4:D:218:GLU:HG3	2.14	0.48
4:D:248:PRO:O	4:D:252:GLU:HG3	2.14	0.48
4:D:647:ARG:NH2	4:D:671:ASN:ND2	2.62	0.48
4:D:721:LYS:O	4:D:722:ARG:C	2.56	0.48
4:D:154:ILE:O	4:D:158:GLU:HB3	2.13	0.48
4:D:706:LEU:HD11	4:D:849:PHE:CB	2.43	0.48
4:D:32:LEU:O	4:D:33:ALA:C	2.57	0.48
4:D:308:TYR:CE2	4:D:734:PRO:HG2	2.49	0.48
4:D:652:GLU:O	4:D:657:PRO:HD3	2.14	0.48
1:T:130:DG:H2''	1:T:129:DC:H6	1.78	0.48
4:D:307:ARG:HG2	4:D:736:TRP:CH2	2.48	0.48
4:D:358:GLU:CD	4:D:358:GLU:H	2.22	0.48
1:T:112:DG:H2'	4:D:57:ARG:HH12	1.77	0.47
4:D:585:ASP:OD1	4:D:613:THR:HG21	2.14	0.47
1:T:130:DG:H2''	1:T:129:DC:C6	2.49	0.47
4:D:274:PRO:HB3	4:D:325:ASN:HD22	1.78	0.47
4:D:720:ARG:NH1	4:D:854:HIS:HA	2.29	0.47
4:D:783:VAL:O	4:D:786:GLN:HB2	2.14	0.47
4:D:849:PHE:CE2	4:D:861:MET:HE3	2.49	0.47
4:D:111:PRO:O	4:D:114:VAL:HB	2.14	0.47
4:D:150:ARG:C	4:D:152:GLY:H	2.23	0.47
4:D:611:LEU:CD1	4:D:619:GLN:HE22	2.25	0.47
4:D:36:GLN:HE22	4:D:271:CYS:HA	1.78	0.47
4:D:89:PHE:C	4:D:91:GLU:N	2.72	0.47
4:D:667:PHE:O	4:D:668:THR:C	2.58	0.47
1:T:119:DT:C2'	1:T:118:DC:OP2	2.57	0.47
4:D:13:ASP:CB	4:D:16:LEU:HD13	2.42	0.47
4:D:15:GLU:HA	4:D:15:GLU:OE1	2.14	0.47
4:D:51:PHE:CD2	4:D:262:ALA:HB2	2.49	0.47
4:D:163:LYS:O	4:D:165:ASN:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:551:ARG:HB2	4:D:868:GLY:H	1.78	0.47
4:D:711:LYS:HE2	4:D:716:GLY:O	2.14	0.47
4:D:738:GLU:O	4:D:738:GLU:HG3	2.14	0.47
4:D:822:ALA:O	4:D:825:PHE:HB3	2.14	0.47
4:D:100:PRO:O	4:D:102:ALA:N	2.43	0.47
4:D:183:MET:HE1	4:D:186:VAL:HG11	1.97	0.47
4:D:409:ALA:O	4:D:410:ASN:CB	2.63	0.47
4:D:767:SER:O	4:D:768:GLU:CB	2.61	0.47
4:D:828:VAL:CG2	4:D:883:ALA:HA	2.43	0.47
4:D:344:TRP:O	4:D:345:LYS:C	2.57	0.47
4:D:632:ARG:HH11	4:D:632:ARG:HG3	1.79	0.47
4:D:219:MET:HA	4:D:222:GLU:HB3	1.97	0.47
4:D:169:GLN:O	4:D:170:LEU:C	2.57	0.46
4:D:298:ARG:HG3	4:D:420:MET:O	2.15	0.46
4:D:473:VAL:CG1	4:D:477:GLU:HB3	2.44	0.46
4:D:720:ARG:HG3	4:D:720:ARG:NH1	2.30	0.46
4:D:828:VAL:HG11	4:D:882:PHE:O	2.16	0.46
4:D:120:LYS:HD2	4:D:752:LEU:HD23	1.97	0.46
4:D:439:MET:HE3	4:D:443:LEU:CD2	2.45	0.46
4:D:450:LYS:HZ3	4:D:820:ASP:CG	2.22	0.46
4:D:99:ARG:O	4:D:101:THR:N	2.41	0.46
4:D:551:ARG:C	4:D:870:LEU:HB3	2.40	0.46
4:D:13:ASP:CB	4:D:16:LEU:HD22	2.43	0.46
4:D:642:LYS:HA	4:D:682:TRP:CZ3	2.50	0.46
4:D:720:ARG:HH12	4:D:858:LEU:HD12	1.81	0.46
4:D:113:ALA:O	4:D:117:ILE:HG13	2.15	0.46
4:D:278:TRP:CD2	4:D:284:GLY:HA3	2.50	0.46
4:D:571:TYR:CE2	4:D:631:LYS:NZ	2.82	0.46
1:T:119:DT:H2'	1:T:119:DT:O5'	2.16	0.46
4:D:224:THR:OG1	4:D:225:GLY:N	2.49	0.46
4:D:99:ARG:HD3	4:D:103:PHE:CD2	2.51	0.46
4:D:349:VAL:O	4:D:350:GLU:C	2.59	0.46
4:D:398:LEU:C	4:D:398:LEU:HD23	2.40	0.46
4:D:491:ALA:HB1	4:D:499:ASN:OD1	2.15	0.46
4:D:36:GLN:CG	4:D:273:VAL:HG22	2.46	0.46
4:D:416:PHE:CE1	4:D:433:ASN:HA	2.51	0.46
4:D:534:LEU:HD12	4:D:818:PRO:HA	1.98	0.46
1:T:120:DT:C2'	1:T:119:DT:OP2	2.64	0.46
4:D:35:GLU:O	4:D:39:LEU:HB2	2.15	0.46
4:D:117:ILE:HA	4:D:752:LEU:CD2	2.45	0.46
4:D:855:GLU:CD	4:D:856:SER:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:164:LYS:C	4:D:166:VAL:N	2.72	0.45
4:D:802:TYR:OH	4:D:826:LYS:HD3	2.16	0.45
4:D:178:TYR:C	4:D:180:LYS:N	2.73	0.45
4:D:551:ARG:O	4:D:870:LEU:HB3	2.16	0.45
4:D:154:ILE:O	4:D:154:ILE:HG12	2.16	0.45
4:D:729:THR:OG1	4:D:733:PHE:HB3	2.16	0.45
4:D:59:LEU:C	4:D:61:ALA:N	2.74	0.45
4:D:562:LEU:HD21	4:D:870:LEU:HD12	1.99	0.45
4:D:689:VAL:HG12	4:D:692:ALA:HB3	1.97	0.45
4:D:151:PHE:CD1	4:D:151:PHE:N	2.83	0.45
4:D:361:PRO:HG2	4:D:385:TYR:HE1	1.80	0.45
4:D:705:LEU:HD12	4:D:861:MET:HE2	1.98	0.45
3:R:4:C:H3'	3:R:4:C:H6	1.82	0.45
4:D:154:ILE:CD1	4:D:158:GLU:HG2	2.45	0.45
4:D:566:THR:CG2	4:D:568:GLN:OE1	2.64	0.45
4:D:664:GLY:O	4:D:666:MET:N	2.41	0.45
1:T:117:DG:H5'	1:T:117:DG:H8	1.82	0.45
4:D:107:GLN:HA	4:D:107:GLN:OE1	2.16	0.45
4:D:274:PRO:HA	4:D:275:PRO:HD3	1.90	0.45
4:D:452:ILE:HG23	4:D:453:GLY:N	2.32	0.45
4:D:664:GLY:C	4:D:666:MET:H	2.21	0.45
4:D:757:LEU:HD23	4:D:758:GLN:H	1.81	0.45
4:D:337:VAL:CG2	4:D:338:ALA:N	2.79	0.45
4:D:13:ASP:OD1	4:D:16:LEU:HD13	2.17	0.45
4:D:133:THR:HG22	4:D:243:THR:CG2	2.34	0.45
4:D:473:VAL:HG13	4:D:477:GLU:HB3	1.98	0.45
4:D:473:VAL:N	4:D:567:VAL:HG11	2.32	0.45
2:N:16:DT:C3'	4:D:378:LYS:HD3	2.46	0.45
4:D:134:VAL:HG23	4:D:135:GLN:N	2.32	0.45
4:D:184:GLN:HG3	4:D:185:VAL:H	1.80	0.45
4:D:24:LEU:HD21	4:D:287:TRP:CD2	2.52	0.44
4:D:311:VAL:HG11	4:D:734:PRO:HG3	1.98	0.44
4:D:339:ASN:ND2	4:D:406:ASN:HD21	2.14	0.44
4:D:152:GLY:HA2	4:D:750:MET:SD	2.57	0.44
2:N:20:DT:C2	4:D:647:ARG:NH1	2.86	0.44
4:D:110:LYS:HE3	4:D:113:ALA:HB2	2.00	0.44
4:D:463:HIS:CB	4:D:534:LEU:HD22	2.46	0.44
4:D:637:LEU:CD2	4:D:689:VAL:HB	2.48	0.44
4:D:690:VAL:O	4:D:691:ALA:C	2.58	0.44
4:D:53:LYS:NZ	4:D:57:ARG:HG2	2.32	0.44
4:D:82:ILE:HG13	4:D:86:ASN:OD1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:592:ASN:ND2	4:D:592:ASN:H	2.14	0.44
4:D:705:LEU:HD22	4:D:858:LEU:CD2	2.48	0.44
4:D:706:LEU:HD11	4:D:849:PHE:HB2	2.00	0.44
3:R:1:3DA:H5'1	7:D:904:HOH:O	2.18	0.44
4:D:686:SER:C	4:D:688:THR:H	2.26	0.44
4:D:723:CYS:SG	4:D:853:LEU:HD13	2.58	0.44
2:N:26:DA:H2''	2:N:27:DC:O5'	2.18	0.44
4:D:110:LYS:HB2	4:D:113:ALA:HB2	1.99	0.44
4:D:465:ALA:CB	4:D:478:ARG:HB3	2.48	0.44
4:D:473:VAL:CG2	4:D:474:PRO:HD2	2.41	0.44
4:D:807:PHE:HB3	4:D:809:LEU:HD21	2.00	0.44
4:D:71:LYS:HD2	4:D:75:THR:HG23	1.99	0.43
1:T:120:DT:H71	4:D:632:ARG:HH21	1.82	0.43
2:N:28:DG:H1'	2:N:29:DG:C5	2.53	0.43
4:D:623:TYR:HA	4:D:666:MET:HE1	2.00	0.43
4:D:361:PRO:HG3	4:D:384:VAL:HB	1.98	0.43
4:D:826:LYS:NZ	4:D:826:LYS:HB3	2.32	0.43
4:D:623:TYR:HD1	4:D:666:MET:HE1	1.83	0.43
4:D:739:TYR:N	4:D:774:GLN:NE2	2.52	0.43
4:D:752:LEU:HD12	4:D:752:LEU:N	2.33	0.43
4:D:855:GLU:OE1	4:D:856:SER:N	2.52	0.43
4:D:149:ALA:O	4:D:153:ARG:HB2	2.19	0.43
4:D:623:TYR:CD2	4:D:624:GLY:N	2.86	0.43
4:D:779:ALA:HB3	4:D:780:PRO:CD	2.48	0.43
4:D:69:ALA:O	4:D:257:ARG:HG2	2.17	0.43
4:D:118:THR:O	4:D:122:THR:HG23	2.18	0.43
4:D:377:TRP:C	4:D:379:ARG:HB2	2.44	0.43
4:D:647:ARG:HH21	4:D:671:ASN:HD21	1.65	0.43
4:D:162:PHE:C	4:D:164:LYS:N	2.75	0.43
4:D:245:GLU:O	4:D:245:GLU:HG3	2.18	0.43
4:D:275:PRO:HB2	4:D:324:GLN:CG	2.44	0.43
4:D:125:CYS:HA	4:D:128:SER:HB3	2.00	0.43
4:D:623:TYR:HA	4:D:666:MET:CE	2.49	0.43
4:D:723:CYS:CB	4:D:853:LEU:HD13	2.48	0.43
1:T:119:DT:C2'	1:T:119:DT:O5'	2.66	0.43
4:D:13:ASP:HB3	4:D:16:LEU:CD1	2.48	0.43
4:D:36:GLN:HG3	4:D:273:VAL:HG22	2.01	0.43
4:D:433:ASN:HB2	4:D:434:PRO:CD	2.49	0.43
4:D:452:ILE:N	4:D:528:TYR:O	2.42	0.43
4:D:698:TRP:HZ3	4:D:845:PHE:HD2	1.67	0.43
2:N:19:DG:H2''	2:N:20:DT:C7	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:58:GLN:OE1	4:D:58:GLN:HA	2.19	0.42
4:D:169:GLN:O	4:D:169:GLN:CD	2.61	0.42
4:D:349:VAL:HG13	4:D:508:PRO:HG3	2.01	0.42
4:D:357:ARG:HB3	4:D:358:GLU:OE2	2.19	0.42
4:D:402:LEU:HD12	4:D:402:LEU:HA	1.78	0.42
4:D:613:THR:O	4:D:614:LYS:HB3	2.18	0.42
4:D:852:GLN:O	4:D:853:LEU:HB2	2.19	0.42
4:D:86:ASN:C	4:D:88:TRP:N	2.75	0.42
4:D:470:VAL:HG21	4:D:481:PHE:CG	2.53	0.42
4:D:670:PRO:O	4:D:673:ALA:HB3	2.19	0.42
4:D:854:HIS:HD2	4:D:858:LEU:HD13	1.84	0.42
4:D:34:ARG:HH11	4:D:34:ARG:HG2	1.83	0.42
4:D:102:ALA:O	4:D:103:PHE:C	2.62	0.42
4:D:215:ARG:CG	4:D:219:MET:HE3	2.39	0.42
4:D:13:ASP:OD2	4:D:14:ILE:N	2.52	0.42
4:D:218:GLU:C	4:D:220:LEU:H	2.27	0.42
4:D:689:VAL:CG1	4:D:692:ALA:HB3	2.50	0.42
4:D:744:GLN:CB	4:D:756:ARG:HB3	2.48	0.42
4:D:50:ARG:NE	4:D:267:MET:HE2	2.34	0.42
4:D:416:PHE:CE2	4:D:434:PRO:HD3	2.55	0.42
4:D:490:MET:SD	4:D:522:GLN:HG3	2.59	0.42
4:D:669:GLN:NE2	4:D:672:GLN:NE2	2.67	0.42
4:D:146:GLU:O	4:D:147:ASP:HB2	2.20	0.42
4:D:421:ASP:CG	4:D:423:ARG:NH1	2.77	0.42
4:D:450:LYS:O	4:D:451:PRO:C	2.61	0.42
4:D:852:GLN:O	4:D:853:LEU:CB	2.67	0.42
4:D:78:LEU:HD21	4:D:755:PHE:CD2	2.55	0.42
4:D:449:GLY:O	4:D:450:LYS:HG2	2.20	0.42
4:D:705:LEU:O	4:D:720:ARG:NH2	2.48	0.42
4:D:828:VAL:HG13	4:D:882:PHE:O	2.19	0.42
4:D:298:ARG:N	4:D:420:MET:O	2.52	0.42
4:D:537:ASP:O	4:D:882:PHE:CD1	2.71	0.42
4:D:585:ASP:HB3	4:D:613:THR:CG2	2.49	0.42
4:D:613:THR:CG2	4:D:614:LYS:H	2.16	0.42
4:D:645:GLY:O	4:D:649:GLN:HG3	2.20	0.42
4:D:655:ILE:O	4:D:659:ILE:HG13	2.19	0.42
4:D:746:ARG:HB3	4:D:756:ARG:HG2	2.02	0.42
1:T:114:DG:O6	3:R:8:A:N6	2.53	0.42
4:D:115:ALA:O	4:D:119:ILE:HG13	2.20	0.42
4:D:122:THR:HG21	4:D:220:LEU:HD22	2.01	0.42
4:D:165:ASN:OD1	4:D:168:GLU:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:328:TRP:CH2	4:D:434:PRO:HB3	2.55	0.42
4:D:385:TYR:HD1	4:D:385:TYR:H	1.67	0.42
4:D:517:GLU:HG3	4:D:532:LEU:HB2	2.01	0.42
4:D:624:GLY:O	4:D:625:VAL:C	2.62	0.42
2:N:29:DG:H2''	2:N:30:DC:OP2	2.20	0.41
4:D:52:ARG:HA	4:D:52:ARG:HD3	1.87	0.41
4:D:150:ARG:C	4:D:152:GLY:N	2.76	0.41
4:D:562:LEU:HD21	4:D:870:LEU:CD1	2.50	0.41
4:D:782:PHE:O	4:D:786:GLN:HG2	2.20	0.41
2:N:19:DG:N2	4:D:670:PRO:HD2	2.35	0.41
3:R:7:C:OP1	4:D:169:GLN:HG3	2.19	0.41
4:D:86:ASN:C	4:D:88:TRP:H	2.28	0.41
4:D:161:HIS:HA	4:D:164:LYS:HG2	2.02	0.41
4:D:439:MET:HE3	4:D:443:LEU:HD21	2.01	0.41
4:D:50:ARG:CB	4:D:267:MET:HE3	2.49	0.41
4:D:355:ILE:HB	4:D:356:GLU:OE2	2.21	0.41
4:D:720:ARG:HH22	4:D:858:LEU:HD11	1.84	0.41
4:D:13:ASP:OD2	4:D:13:ASP:C	2.61	0.41
4:D:48:GLU:HG3	4:D:262:ALA:CB	2.49	0.41
4:D:298:ARG:NH2	4:D:419:ASN:ND2	2.35	0.41
4:D:324:GLN:CB	4:D:418:TYR:HD1	2.33	0.41
4:D:109:ILE:CG2	4:D:149:ALA:HA	2.50	0.41
4:D:146:GLU:C	4:D:148:GLU:N	2.78	0.41
4:D:188:ALA:O	4:D:189:ASP:C	2.63	0.41
4:D:488:ASN:HB3	4:D:501:TRP:CZ3	2.56	0.41
4:D:750:MET:O	4:D:751:PHE:CB	2.67	0.41
1:T:129:DC:H2''	1:T:128:DC:C5	2.56	0.41
1:T:120:DT:H5'	4:D:641:SER:HA	2.03	0.41
4:D:40:GLU:OE1	4:D:288:ALA:N	2.48	0.41
4:D:359:GLU:O	4:D:360:LEU:O	2.39	0.41
3:R:6:G:O2'	4:D:390:ALA:HA	2.21	0.41
4:D:547:SER:O	4:D:551:ARG:N	2.54	0.41
4:D:720:ARG:NH1	4:D:858:LEU:CD1	2.82	0.41
4:D:99:ARG:HA	4:D:100:PRO:HD3	1.84	0.41
4:D:159:ALA:O	4:D:160:LYS:HB2	2.21	0.41
4:D:622:ALA:O	4:D:623:TYR:O	2.38	0.41
4:D:646:PHE:N	4:D:646:PHE:CD2	2.88	0.41
4:D:663:LYS:HD2	4:D:663:LYS:N	2.35	0.41
4:D:882:PHE:C	4:D:883:ALA:O	2.61	0.41
3:R:6:G:O2'	3:R:5:G:H5'	2.20	0.41
4:D:18:ALA:O	4:D:20:PRO:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:81:MET:HE3	4:D:85:ILE:HD11	2.03	0.41
4:D:109:ILE:HG21	4:D:149:ALA:HA	2.02	0.41
4:D:171:ASN:OD1	4:D:179:LYS:HB3	2.21	0.41
4:D:278:TRP:CD1	4:D:324:GLN:HE22	2.39	0.41
4:D:299:THR:OG1	4:D:305:LEU:HB2	2.20	0.41
4:D:631:LYS:O	4:D:632:ARG:C	2.64	0.41
4:D:854:HIS:CG	4:D:855:GLU:H	2.38	0.41
4:D:36:GLN:HE21	4:D:272:VAL:HG22	1.85	0.41
4:D:111:PRO:HG2	4:D:112:GLU:H	1.85	0.41
4:D:269:GLN:HB3	4:D:270:PRO:HD2	2.01	0.41
4:D:690:VAL:CG2	4:D:691:ALA:H	2.32	0.41
3:R:7:C:H5'	4:D:172:LYS:CE	2.52	0.40
4:D:118:THR:CG2	4:D:220:LEU:HD13	2.49	0.40
4:D:156:ASP:OD2	4:D:157:LEU:HD23	2.22	0.40
4:D:307:ARG:HG2	4:D:736:TRP:CZ3	2.55	0.40
4:D:485:ASN:O	4:D:486:HIS:C	2.63	0.40
4:D:668:THR:O	4:D:669:GLN:CB	2.69	0.40
4:D:725:VAL:HG11	4:D:778:ILE:HD13	2.03	0.40
4:D:737:GLN:HE22	4:D:778:ILE:N	2.19	0.40
4:D:860:LYS:HA	4:D:860:LYS:HD3	1.87	0.40
1:T:120:DT:OP2	4:D:641:SER:HA	2.21	0.40
4:D:88:TRP:CD2	4:D:219:MET:HE1	2.56	0.40
4:D:671:ASN:O	4:D:672:GLN:HB2	2.21	0.40
4:D:148:GLU:CD	4:D:749:LEU:HB3	2.46	0.40
4:D:552:ASP:CG	4:D:555:GLY:H	2.29	0.40
4:D:664:GLY:C	4:D:666:MET:N	2.80	0.40
4:D:683:GLU:O	4:D:687:VAL:HG13	2.21	0.40
4:D:749:LEU:O	4:D:750:MET:C	2.64	0.40
2:N:22:DG:H2''	2:N:23:DC:C5	2.57	0.40
4:D:497:LEU:H	4:D:497:LEU:CD1	2.24	0.40
4:D:160:LYS:HB2	4:D:160:LYS:HZ3	1.86	0.40
4:D:164:LYS:C	4:D:166:VAL:H	2.29	0.40
4:D:360:LEU:HA	4:D:361:PRO:HD3	1.90	0.40
4:D:361:PRO:HB3	4:D:382:ALA:HA	2.03	0.40
4:D:433:ASN:ND2	4:D:435:GLN:HB2	2.37	0.40
4:D:881:ALA:O	4:D:882:PHE:HB2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	D	822/883 (93%)	669 (81%)	109 (13%)	44 (5%)	1 2

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	226	MET
4	D	350	GLU
4	D	360	LEU
4	D	378	LYS
4	D	379	ARG
4	D	590	THR
4	D	623	TYR
4	D	767	SER
4	D	854	HIS
4	D	62	GLY
4	D	100	PRO
4	D	158	GLU
4	D	164	LYS
4	D	168	GLU
4	D	224	THR
4	D	359	GLU
4	D	625	VAL
4	D	631	LYS
4	D	751	PHE
4	D	857	GLN
4	D	83	ALA
4	D	90	GLU
4	D	106	LEU
4	D	150	ARG
4	D	204	TRP
4	D	225	GLY
4	D	309	GLU
4	D	668	THR

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Mol	Chain	Res	Type
4	D	764	ASN
4	D	852	GLN
4	D	174	VAL
4	D	183	MET
4	D	200	ALA
4	D	357	ARG
4	D	665	LEU
4	D	669	GLN
4	D	768	GLU
4	D	63	GLU
4	D	859	ASP
4	D	882	PHE
4	D	111	PRO
4	D	594	VAL
4	D	20	PRO
4	D	624	GLY

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	
4	D	683/729 (94%)	625 (92%)	58 (8%)	10	25

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	19	ILE
4	D	36	GLN
4	D	50	ARG
4	D	57	ARG
4	D	104	GLN
4	D	107	GLN
4	D	143	ARG
4	D	160	LYS
4	D	167	GLU
4	D	169	GLN

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Mol	Chain	Res	Type
4	D	206	LYS
4	D	242	GLU
4	D	276	LYS
4	D	292	ARG
4	D	310	ASP
4	D	318	LYS
4	D	324	GLN
4	D	329	LYS
4	D	333	LYS
4	D	337	VAL
4	D	339	ASN
4	D	341	ILE
4	D	351	ASP
4	D	352	ILE
4	D	356	GLU
4	D	358	GLU
4	D	393	SER
4	D	403	GLU
4	D	419	ASN
4	D	423	ARG
4	D	433	ASN
4	D	443	LEU
4	D	473	VAL
4	D	480	LYS
4	D	488	ASN
4	D	497	LEU
4	D	514	PHE
4	D	527	SER
4	D	561	LEU
4	D	566	THR
4	D	567	VAL
4	D	588	ASN
4	D	592	ASN
4	D	628	SER
4	D	666	MET
4	D	743	ILE
4	D	747	LEU
4	D	757	LEU
4	D	773	LYS
4	D	816	THR
4	D	826	LYS
4	D	838	SER

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Mol	Chain	Res	Type
4	D	842	LEU
4	D	855	GLU
4	D	857	GLN
4	D	859	ASP
4	D	874	ASP
4	D	876	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	36	GLN
4	D	104	GLN
4	D	165	ASN
4	D	321	ASN
4	D	325	ASN
4	D	346	HIS
4	D	404	GLN
4	D	406	ASN
4	D	419	ASN
4	D	433	ASN
4	D	463	HIS
4	D	488	ASN
4	D	522	GLN
4	D	529	ASN
4	D	588	ASN
4	D	592	ASN
4	D	619	GLN
4	D	648	GLN
4	D	649	GLN
4	D	669	GLN
4	D	672	GLN
4	D	697	ASN
4	D	737	GLN
4	D	762	ASN
4	D	774	GLN
4	D	781	ASN
4	D	786	GLN
4	D	790	HIS
4	D	811	HIS
4	D	848	GLN
4	D	852	GLN
4	D	871	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	R	8/10 (80%)	2 (25%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	R	8	A
3	R	2	A

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue 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	3DA	R	1	5,1,3	19,23,24	0.32	0	25,33,36	0.41	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	3DA	R	1	5,1,3	-	1/7/21/22	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	R	1	3DA	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	1	3DA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	POP	D	901	-	6,8,8	1.14	0	12,13,13	0.82	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
6	POP	D	901	-	-	0/6/6/6	-

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, 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	T	21/21 (100%)	2.10	14 (66%) 0 0	43, 124, 149, 149	0
2	N	17/17 (100%)	2.42	15 (88%) 0 0	144, 148, 149, 150	0
3	R	9/10 (90%)	2.14	6 (66%) 0 0	76, 95, 128, 135	0
4	D	828/883 (93%)	1.08	148 (17%) 3 3	24, 61, 105, 127	0
All	All	875/931 (93%)	1.14	183 (20%) 2 2	24, 63, 110, 150	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	377	TRP	6.9
4	D	177	VAL	6.8
4	D	83	ALA	6.8
4	D	106	LEU	6.7
4	D	182	PHE	5.5
4	D	148	GLU	4.9
4	D	853	LEU	4.8
4	D	159	ALA	4.7
4	D	174	VAL	4.6
4	D	12	SER	4.6
4	D	743	ILE	4.4
4	D	105	PHE	4.4
4	D	209	SER	4.3
4	D	185	VAL	4.3
4	D	204	TRP	4.2
4	D	383	ALA	4.0
4	D	166	VAL	4.0
4	D	252	GLU	3.8
4	D	152	GLY	3.8
4	D	210	ILE	3.7
4	D	877	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
4	D	661	SER	3.7
4	D	141	ILE	3.7
2	N	29	DG	3.7
4	D	178	TYR	3.7
4	D	200	ALA	3.6
4	D	206	LYS	3.6
4	D	761	ILE	3.6
4	D	137	VAL	3.6
4	D	102	ALA	3.6
1	T	114	DG	3.5
4	D	17	ALA	3.5
4	D	760	THR	3.5
4	D	131	ASN	3.5
4	D	160	LYS	3.5
4	D	594	VAL	3.4
4	D	132	THR	3.3
1	T	115	DC	3.3
4	D	157	LEU	3.3
4	D	61	ALA	3.3
4	D	755	PHE	3.3
4	D	766	ASP	3.2
4	D	126	LEU	3.1
4	D	854	HIS	3.1
1	T	130	DG	3.1
4	D	665	LEU	3.1
2	N	18	DC	3.0
4	D	725	VAL	3.0
4	D	136	ALA	3.0
4	D	360	LEU	3.0
4	D	95	LYS	3.0
4	D	190	MET	3.0
2	N	17	DA	3.0
4	D	354	ALA	3.0
4	D	89	PHE	3.0
4	D	151	PHE	3.0
4	D	162	PHE	3.0
4	D	168	GLU	2.9
4	D	748	ASN	2.9
4	D	609	VAL	2.9
4	D	154	ILE	2.9
4	D	244	ILE	2.9
4	D	659	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
4	D	745	THR	2.9
4	D	186	VAL	2.8
4	D	389	LYS	2.8
4	D	245	GLU	2.8
3	R	7	C	2.8
4	D	171	ASN	2.8
4	D	858	LEU	2.8
2	N	14	DT	2.7
4	D	87	ASP	2.7
2	N	26	DA	2.7
4	D	191	LEU	2.7
4	D	92	VAL	2.7
1	T	128	DC	2.7
4	D	749	LEU	2.7
4	D	130	ASP	2.7
4	D	670	PRO	2.7
4	D	119	ILE	2.6
4	D	217	ILE	2.6
4	D	587	ILE	2.6
1	T	110	DT	2.6
4	D	291	ARG	2.6
4	D	654	THR	2.6
4	D	744	GLN	2.6
4	D	220	LEU	2.6
4	D	96	ARG	2.6
4	D	193	LYS	2.6
4	D	97	GLY	2.6
2	N	30	DC	2.6
4	D	219	MET	2.6
4	D	16	LEU	2.6
4	D	229	LEU	2.6
4	D	90	GLU	2.6
4	D	175	GLY	2.6
1	T	124	DC	2.5
3	R	3	G	2.5
4	D	81	MET	2.5
4	D	380	ALA	2.5
4	D	170	LEU	2.5
4	D	873	ARG	2.5
4	D	103	PHE	2.5
4	D	85	ILE	2.5
4	D	384	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
3	R	2	A	2.4
4	D	592	ASN	2.4
4	D	246	LEU	2.4
4	D	156	ASP	2.4
4	D	201	TRP	2.4
1	T	126	DT	2.4
1	T	111	DT	2.4
4	D	65	ALA	2.4
4	D	378	LYS	2.4
4	D	497	LEU	2.4
1	T	127	DG	2.4
1	T	112	DG	2.4
4	D	88	TRP	2.4
4	D	492	CYS	2.4
2	N	16	DT	2.4
4	D	161	HIS	2.4
2	N	19	DG	2.4
4	D	653	ASP	2.4
4	D	183	MET	2.4
4	D	742	PRO	2.4
4	D	663	LYS	2.3
1	T	129	DC	2.3
2	N	27	DC	2.3
4	D	107	GLN	2.3
2	N	23	DC	2.3
4	D	55	PHE	2.3
4	D	385	TYR	2.3
4	D	590	THR	2.3
4	D	631	LYS	2.3
4	D	764	ASN	2.3
4	D	64	VAL	2.3
4	D	188	ALA	2.3
2	N	22	DG	2.3
4	D	250	TYR	2.3
4	D	657	PRO	2.3
4	D	14	ILE	2.2
4	D	503	ALA	2.2
1	T	113	DT	2.2
2	N	20	DT	2.2
2	N	24	DG	2.2
4	D	212	VAL	2.2
4	D	205	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
4	D	211	HIS	2.2
4	D	382	ALA	2.2
4	D	153	ARG	2.2
4	D	82	ILE	2.2
4	D	176	HIS	2.2
4	D	249	GLU	2.2
2	N	21	DT	2.2
4	D	674	ALA	2.2
4	D	508	PRO	2.2
4	D	146	GLU	2.1
1	T	125	DG	2.1
4	D	127	THR	2.1
4	D	668	THR	2.1
4	D	747	LEU	2.1
4	D	62	GLY	2.1
4	D	142	GLY	2.1
4	D	18	ALA	2.1
4	D	224	THR	2.1
4	D	180	LYS	2.1
2	N	28	DG	2.1
3	R	6	G	2.1
4	D	227	VAL	2.1
4	D	849	PHE	2.1
4	D	288	ALA	2.1
4	D	361	PRO	2.1
4	D	254	ILE	2.1
4	D	629	VAL	2.1
4	D	552	ASP	2.1
4	D	192	SER	2.1
3	R	8	A	2.1
4	D	359	GLU	2.0
4	D	754	GLN	2.0
3	R	10	A	2.0
1	T	122	DC	2.0
4	D	243	THR	2.0
4	D	769	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	3DA	R	1	21/22	0.90	0.15	32,48,79,83	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	POP	D	901	9/9	0.63	0.15	144,145,145,145	0
5	MG	D	903	1/1	0.87	0.08	61,61,61,61	0
5	MG	R	902	1/1	0.98	0.04	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.