



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 04:47 PM UTC

PDB ID : 3HL2 / pdb_00003hl2
Title : The crystal structure of the human SepSecS-tRNA^{Sec} complex
Authors : Palioura, S.; Steitz, T.A.; Soll, D.; Simonovic, M.
Deposited on : 2009-05-26
Resolution : 2.81 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)
Xtrriage (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

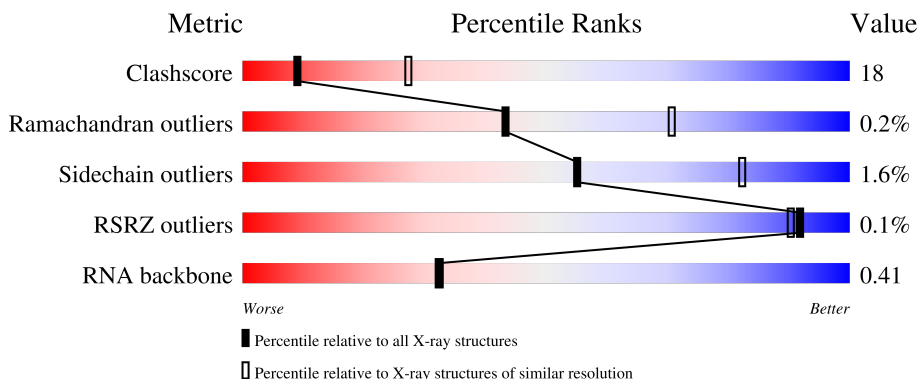
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)
RNA backbone	3983	1142 (3.04-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	A	501	 64% 22% 12% 2%
1	B	501	 63% 25% 12% 2%
1	C	501	 65% 23% 11% 2%
1	D	501	 67% 20% 12% 2%
2	E	90	 19% 67% 9% 2%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 17628 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.

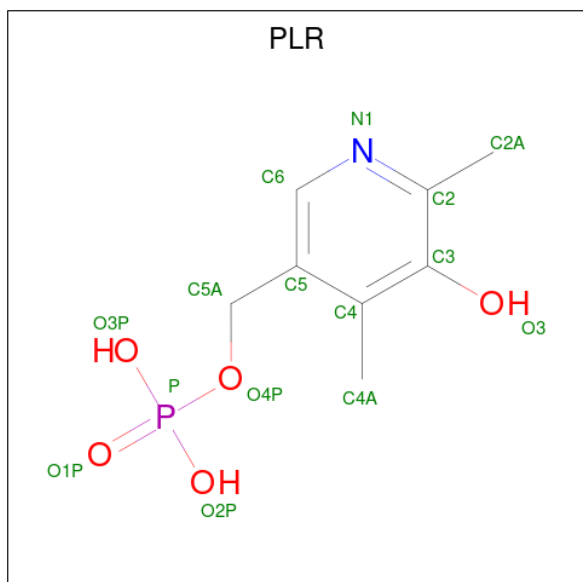
- Molecule 1 is a protein called O-phosphoseryl-tRNA(Sec) selenium transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	441	Total 3426	C 2170	N 602	O 628	S 26	0	6	0
1	B	443	Total 3432	C 2179	N 605	O 621	S 27	0	5	0
1	C	445	Total 3438	C 2175	N 606	O 630	S 27	0	3	0
1	D	441	Total 3411	C 2166	N 602	O 617	S 26	0	6	0

- Molecule 2 is a RNA chain called tRNA^{Sec}.

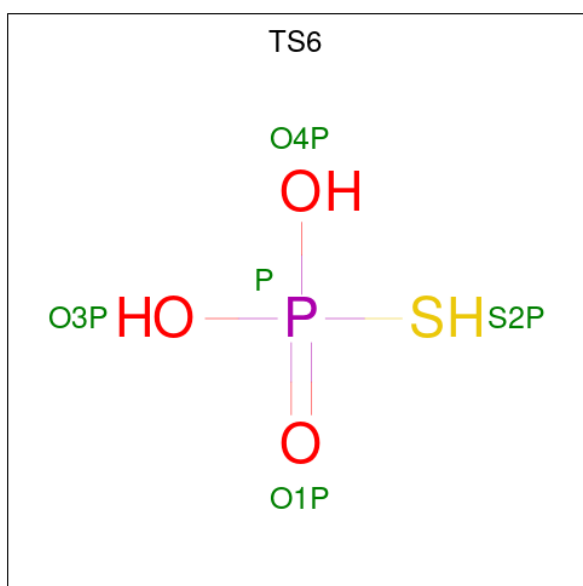
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	E	82	Total 3492	C 1554	N 608	O 1166	P 164	0	82	0

- Molecule 3 is (5-HYDROXY-4,6-DIMETHYLPYRIDIN-3-YL)METHYL DIHYDROGEN PHOSPHATE (CCD ID: PLR) (formula: C₈H₁₂NO₅P).



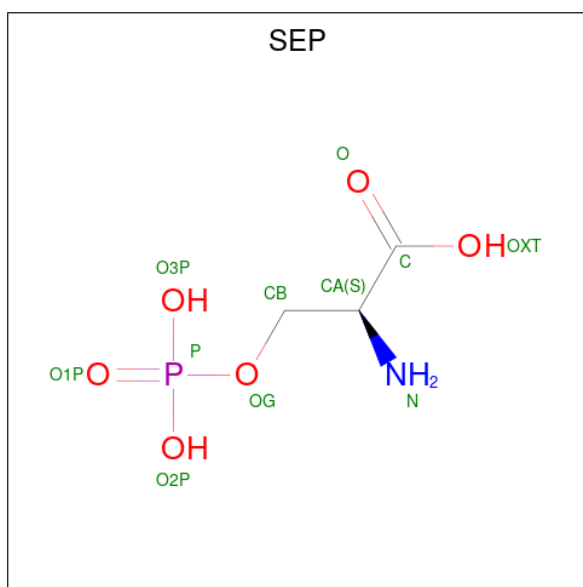
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is Monothiophosphate (CCD ID: TS6) (formula: $\text{H}_3\text{O}_3\text{PS}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	O	P	S	0	0
			5	3	1	1		
4	A	1	Total	O	P	S	0	0
			5	3	1	1		
4	C	1	Total	O	P	S	0	0
			5	3	1	1		

- Molecule 5 is PHOSPHOSERINE (CCD ID: SEP) (formula: $\text{C}_3\text{H}_8\text{NO}_6\text{P}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	B	1	22	6	2	12	2	0	1
5	B	1	11	3	1	6	1	0	0
5	D	1	22	6	2	12	2	0	1
5	D	1	11	3	1	6	1	0	0

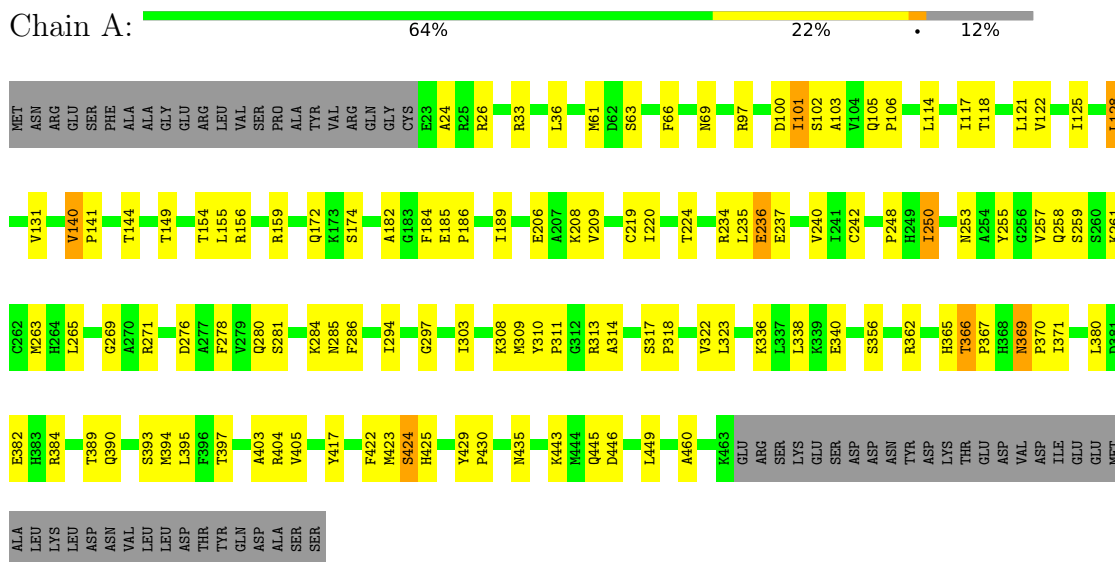
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	71	Total	O	0	0
			71	71		
6	B	87	Total	O	0	0
			87	87		
6	C	67	Total	O	0	0
			67	67		
6	D	58	Total	O	0	0
			58	58		
6	E	5	Total	O	0	0
			5	5		

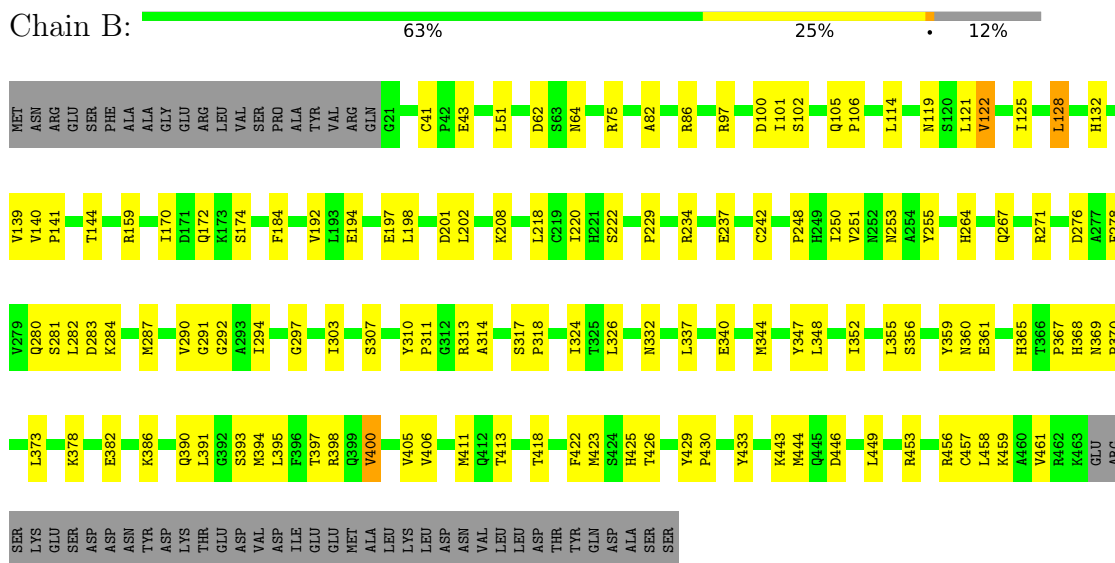
3 Residue-property plots [i](#)

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: O-phosphoseryl-tRNA(Sec) selenium transferase

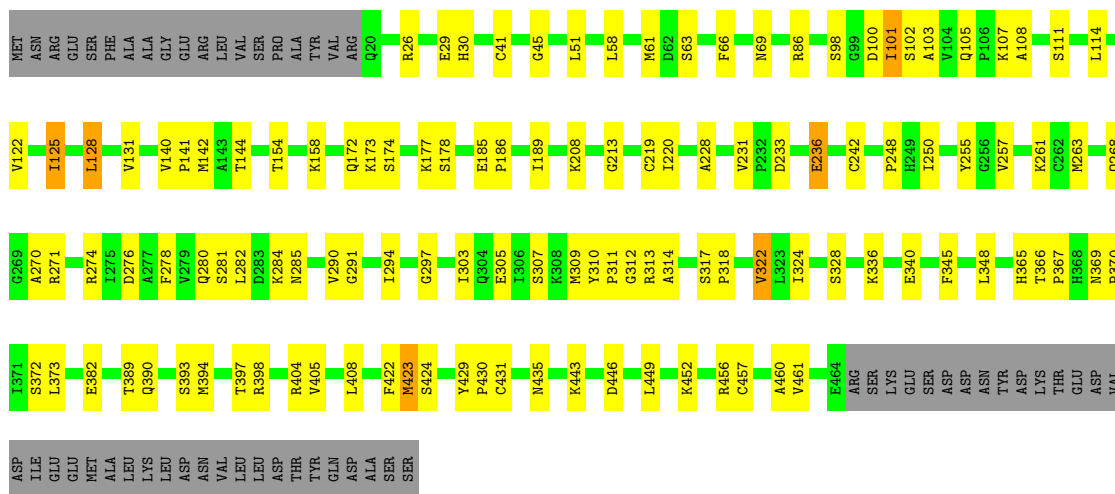


- Molecule 1: O-phosphoseryl-tRNA(Sec) selenium transferase



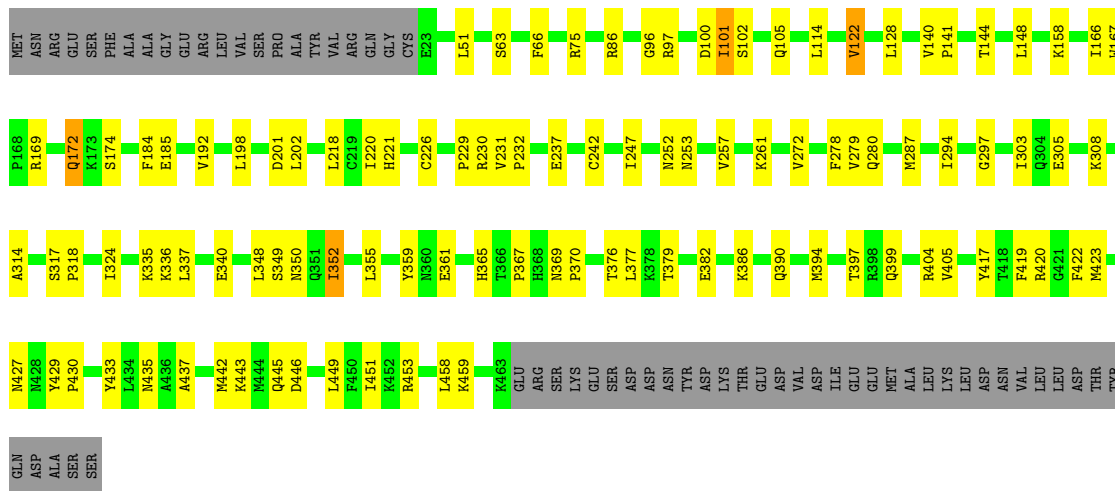
- Molecule 1: O-phosphoseryl-tRNA(Sec) selenium transferase

Chain C:  65% 23% 11%

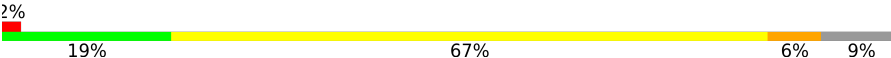


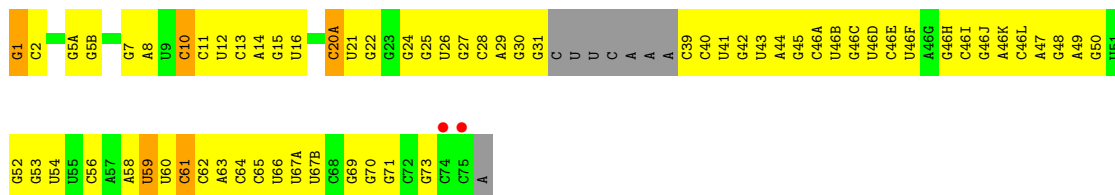
• Molecule 1: O-phosphoseryl-tRNA(Sec) selenium transferase

Chain D:  67% 20% 12%



• Molecule 2: tRNA^{Sec}

Chain E:  19% 67% 6% 9%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	166.82Å 166.82Å 236.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.95 – 2.81 37.95 – 2.81	Depositor EDS
% Data completeness (in resolution range)	97.1 (37.95-2.81) 97.2 (37.95-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.81Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.203 , 0.238 0.193 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	65.4	Xtrriage
Anisotropy	0.234	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.458 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17628	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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: TS6, SEP, PLR

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	0.37	0/3507	0.80	7/4740 (0.1%)
1	B	0.36	0/3509	0.75	3/4741 (0.1%)
1	C	0.37	0/3510	0.79	8/4745 (0.2%)
1	D	0.37	0/3493	0.75	0/4723
2	E	0.32	2/3894 (0.1%)	0.74	10/6058 (0.2%)
All	All	0.36	2/17913 (0.0%)	0.77	28/25007 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1[A]	G	OP3-P	6.05	1.60	1.48
2	E	1[B]	G	OP3-P	6.05	1.60	1.48

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	59[A]	U	N1-C1'-C2'	-7.84	100.24	112.00
2	E	59[B]	U	N1-C1'-C2'	-7.84	100.24	112.00
2	E	61[A]	C	N1-C1'-C2'	-6.23	102.65	112.00
2	E	61[B]	C	N1-C1'-C2'	-6.23	102.65	112.00
1	A	369	ASN	CA-C-N	6.18	125.80	119.56
1	A	369	ASN	C-N-CA	6.18	125.80	119.56
1	A	424	SER	N-CA-C	-6.02	106.27	113.97
1	B	406	VAL	N-CA-C	5.94	114.03	108.15
2	E	10[A]	C	N1-C1'-C2'	-5.60	103.60	112.00
2	E	10[B]	C	N1-C1'-C2'	-5.60	103.60	112.00
2	E	61[A]	C	P-O3'-C3'	-5.59	111.82	120.20
2	E	61[B]	C	P-O3'-C3'	-5.59	111.82	120.20
1	B	159	ARG	CA-C-N	5.56	125.18	119.56
1	B	159	ARG	C-N-CA	5.56	125.18	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	423	MET	CB-CA-C	-5.46	102.20	110.06
1	A	159	ARG	CA-C-N	5.36	125.03	119.56
1	A	159	ARG	C-N-CA	5.36	125.03	119.56
1	C	270	ALA	CA-C-N	5.34	127.38	120.44
1	C	270	ALA	C-N-CA	5.34	127.38	120.44
2	E	20(A)[A]	C	N1-C1'-C2'	-5.32	104.01	112.00
2	E	20(A)[B]	C	N1-C1'-C2'	-5.32	104.01	112.00
1	A	366	THR	CA-C-N	5.24	125.55	119.47
1	A	366	THR	C-N-CA	5.24	125.55	119.47
1	C	213	GLY	CA-C-N	5.15	125.19	119.32
1	C	213	GLY	C-N-CA	5.15	125.19	119.32
1	C	369	ASN	CA-C-N	5.11	125.55	120.04
1	C	369	ASN	C-N-CA	5.11	125.55	120.04
1	C	424	SER	N-CA-C	-5.06	107.15	113.72

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	3426	0	3465	89	0
1	B	3432	0	3468	105	0
1	C	3438	0	3455	94	0
1	D	3411	0	3447	83	0
2	E	3492	0	1728	247	0
3	A	15	0	8	2	0
3	B	15	0	8	1	0
3	C	15	0	8	3	0
3	D	15	0	8	1	0
4	A	10	0	2	0	0
4	C	5	0	1	0	0
5	B	33	0	15	5	0
5	D	33	0	15	5	0
6	A	71	0	0	2	0
6	B	87	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	67	0	0	4	0
6	D	58	0	0	0	0
6	E	5	0	0	0	0
All	All	17628	0	15628	605	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 18.

All (605) 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:D:128:LEU:HD11	1:D:335:LYS:CE	1.74	1.17
2:E:46(C)[A]:G:O2'	2:E:46(D)[A]:U:H5'	1.45	1.15
2:E:46(C)[B]:G:O2'	2:E:46(D)[B]:U:H5'	1.45	1.13
2:E:49[B]:A:H4'	2:E:50[B]:G:H5'	1.16	1.13
2:E:46(C)[B]:G:C2'	2:E:46(D)[B]:U:H5'	1.80	1.11
2:E:46(C)[A]:G:C2'	2:E:46(D)[A]:U:H5'	1.80	1.10
2:E:49[A]:A:H4'	2:E:50[A]:G:H5'	1.16	1.09
1:D:128:LEU:HD11	1:D:335:LYS:HE3	1.40	1.04
1:D:278:PHE:CE1	1:D:280:GLN:NE2	2.25	1.03
2:E:46(H)[A]:G:O2'	2:E:46(I)[A]:C:H5'	1.57	1.03
2:E:46(H)[B]:G:O2'	2:E:46(I)[B]:C:H5'	1.57	1.02
2:E:49[A]:A:H4'	2:E:50[A]:G:C5'	1.90	1.02
2:E:49[B]:A:H4'	2:E:50[B]:G:C5'	1.90	1.01
1:D:278:PHE:CD1	1:D:280:GLN:NE2	2.33	0.96
1:D:128:LEU:HD11	1:D:335:LYS:HE2	1.45	0.94
2:E:49[B]:A:C4'	2:E:50[B]:G:H5'	1.98	0.92
2:E:26[B]:U:H2'	2:E:27[B]:G:C8	2.05	0.92
2:E:49[A]:A:C4'	2:E:50[A]:G:H5'	1.98	0.92
1:D:404:ARG:HB3	1:D:435:ASN:HB2	1.49	0.92
2:E:46(K)[A]:A:O2'	2:E:46(L)[A]:C:H5'	1.70	0.91
2:E:26[A]:U:H2'	2:E:27[A]:G:C8	2.05	0.91
2:E:46(K)[B]:A:O2'	2:E:46(L)[B]:C:H5'	1.70	0.90
1:D:278:PHE:HE1	1:D:280:GLN:HE22	0.97	0.89
1:D:287:MET:HE1	1:D:337:LEU:HD13	1.53	0.89
1:B:287:MET:HE1	1:B:337:LEU:HD13	1.52	0.89
2:E:46(C)[A]:G:H2'	2:E:46(D)[A]:U:H5'	1.57	0.86
2:E:46(C)[B]:G:H2'	2:E:46(D)[B]:U:H5'	1.57	0.84
2:E:46(B)[B]:U:H2'	2:E:46(C)[B]:G:H8	1.42	0.84
2:E:46(B)[A]:U:H2'	2:E:46(C)[A]:G:H8	1.42	0.83
2:E:58[A]:A:H4'	2:E:59[A]:U:OP1	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:LEU:HD12	1:A:265:LEU:HB3	1.60	0.82
1:B:297:GLY:HA3	1:B:303:ILE:HD11	1.61	0.82
1:A:261:LYS:HG2	1:A:370:PRO:HG3	1.61	0.81
1:B:141:PRO:HG2	1:B:314:ALA:HB1	1.61	0.81
2:E:58[B]:A:H4'	2:E:59[B]:U:OP1	1.79	0.81
1:D:141:PRO:HG2	1:D:314:ALA:HB1	1.62	0.81
1:B:426:THR:HG22	6:B:519:HOH:O	1.81	0.80
2:E:40[B]:C:H2'	2:E:41[B]:U:C6	2.17	0.80
1:B:278:PHE:HD2	1:B:280:GLN:HE21	1.26	0.80
2:E:12[A]:U:H2'	2:E:13[A]:C:H6	1.47	0.80
1:B:278:PHE:CD2	1:B:280:GLN:NE2	2.50	0.79
2:E:12[B]:U:H2'	2:E:13[B]:C:H6	1.47	0.79
1:D:278:PHE:HE1	1:D:280:GLN:NE2	1.71	0.79
2:E:60[A]:U:H5''	2:E:61[A]:C:OP2	1.82	0.79
2:E:40[A]:C:H2'	2:E:41[A]:U:C6	2.17	0.78
2:E:7[B]:G:H4'	2:E:8[B]:A:OP2	1.83	0.78
2:E:60[B]:U:H5''	2:E:61[B]:C:OP2	1.82	0.78
1:D:297:GLY:HA3	1:D:303:ILE:HD11	1.64	0.77
2:E:7[A]:G:H4'	2:E:8[A]:A:OP2	1.83	0.77
2:E:46(C)[B]:G:O2'	2:E:46(D)[B]:U:C5'	2.30	0.77
2:E:46(B)[B]:U:H2'	2:E:46(C)[B]:G:C8	2.20	0.77
2:E:44[B]:A:H4'	2:E:45[B]:G:OP1	1.84	0.77
2:E:46(A)[A]:C:H2'	2:E:46(B)[A]:U:C6	2.20	0.77
2:E:46(C)[A]:G:O2'	2:E:46(D)[A]:U:C5'	2.30	0.76
2:E:44[A]:A:H4'	2:E:45[A]:G:OP1	1.84	0.76
2:E:46(A)[B]:C:H2'	2:E:46(B)[B]:U:C6	2.20	0.76
1:C:404:ARG:HB3	1:C:435:ASN:HB2	1.68	0.76
2:E:46(B)[A]:U:H2'	2:E:46(C)[A]:G:C8	2.19	0.76
2:E:26[A]:U:H2'	2:E:27[A]:G:H8	1.49	0.76
1:B:119:ASN:HD21	1:B:139:VAL:H	1.32	0.75
1:A:278:PHE:CD2	1:A:280:GLN:NE2	2.54	0.75
2:E:26[B]:U:H2'	2:E:27[B]:G:H8	1.49	0.75
2:E:41[A]:U:H2'	2:E:42[A]:G:C8	2.22	0.75
2:E:41[B]:U:H2'	2:E:42[B]:G:C8	2.22	0.75
1:B:253:ASN:HB3	1:B:280:GLN:HG3	1.70	0.74
2:E:46(H)[A]:G:C2'	2:E:46(I)[A]:C:H5'	2.16	0.74
2:E:46(H)[B]:G:C2'	2:E:46(I)[B]:C:H5'	2.16	0.74
2:E:46(E)[A]:C:H2'	2:E:46(F)[A]:U:H5'	1.71	0.73
1:B:82:ALA:O	1:B:86:ARG:HG2	1.87	0.73
1:D:261[A]:LYS:HD3	1:D:370:PRO:HG3	1.70	0.72
2:E:12[A]:U:H2'	2:E:13[A]:C:C6	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:20(A)[A]:C:O2'	2:E:21[A]:U:H6	1.73	0.72
2:E:46(E)[B]:C:H2'	2:E:46(F)[B]:U:H5'	1.70	0.72
1:A:141:PRO:HG2	1:A:314:ALA:HB1	1.71	0.72
1:D:449:LEU:HD23	1:D:453:ARG:HH21	1.52	0.72
2:E:12[B]:U:H2'	2:E:13[B]:C:C6	2.24	0.72
1:C:452:LYS:HE2	1:C:456:ARG:HH22	1.54	0.71
2:E:40[B]:C:H2'	2:E:41[B]:U:H6	1.55	0.71
1:D:278:PHE:HD1	1:D:280:GLN:NE2	1.87	0.71
1:A:118:THR:OG1	1:A:323:LEU:HB2	1.90	0.71
2:E:59[A]:U:O2'	2:E:60[A]:U:H5'	1.90	0.71
1:B:283:ASP:OD2	1:B:290:VAL:HG22	1.90	0.71
2:E:20(A)[B]:C:O2'	2:E:21[B]:U:H6	1.73	0.71
2:E:59[B]:U:O2'	2:E:60[B]:U:H5'	1.90	0.71
1:A:422:PHE:O	1:A:423:MET:HB2	1.89	0.70
2:E:40[A]:C:H2'	2:E:41[A]:U:H6	1.55	0.70
2:E:47[A]:A:H2'	2:E:48[A]:G:C8	2.27	0.70
1:C:172:GLN:HE21	1:C:174:SER:H	1.39	0.70
2:E:45[B]:G:H2'	2:E:46(A)[B]:C:H5''	1.74	0.69
1:B:119:ASN:ND2	1:B:139:VAL:H	1.90	0.69
1:A:172:GLN:HE21	1:A:174:SER:HB3	1.58	0.69
2:E:39[B]:C:H2'	2:E:40[B]:C:H6	1.58	0.69
2:E:45[A]:G:H2'	2:E:46(A)[A]:C:H5''	1.74	0.69
2:E:46(J)[B]:G:H2'	2:E:46(K)[B]:A:C8	2.28	0.69
2:E:47[B]:A:H2'	2:E:48[B]:G:C8	2.27	0.69
2:E:39[A]:C:H2'	2:E:40[A]:C:H6	1.58	0.68
1:B:394:MET:O	1:B:398:ARG:HD2	1.93	0.68
1:D:365:HIS:CE1	1:D:367:PRO:HG3	2.29	0.68
2:E:39[B]:C:O2'	2:E:40[B]:C:H5'	1.93	0.68
1:A:313:ARG:HD3	6:A:516:HOH:O	1.93	0.68
2:E:39[A]:C:O2'	2:E:40[A]:C:H5'	1.94	0.68
1:A:253:ASN:HD22	1:A:280:GLN:CG	2.06	0.68
1:D:172:GLN:HE21	1:D:174:SER:HB3	1.58	0.68
1:A:253:ASN:HD22	1:A:280:GLN:HG2	1.58	0.68
2:E:46(J)[A]:G:H2'	2:E:46(K)[A]:A:C8	2.28	0.67
1:C:257:VAL:HG23	1:C:280:GLN:HG2	1.76	0.67
2:E:27[A]:G:C6	2:E:44[A]:A:C6	2.83	0.67
1:B:365:HIS:CE1	1:B:367:PRO:HG3	2.30	0.67
1:B:198:LEU:HD22	1:B:426:THR:HG21	1.77	0.67
2:E:27[B]:G:C6	2:E:44[B]:A:C6	2.83	0.67
1:A:36:LEU:HD23	1:A:117:ILE:HD11	1.75	0.67
2:E:46(A)[B]:C:O2	2:E:48[B]:G:N2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:PRO:CA	1:C:274:ARG:HH21	2.09	0.66
2:E:46(K)[A]:A:C2'	2:E:46(L)[A]:C:H5'	2.26	0.66
1:A:144:THR:HB	3:A:1001:PLR:H5A2	1.77	0.66
1:D:158:LYS:HE2	1:D:305:GLU:OE1	1.96	0.65
1:B:234:ARG:HD3	6:B:524:HOH:O	1.97	0.65
1:B:317:SER:HB3	1:B:318:PRO:HD3	1.79	0.65
1:C:423:MET:HG2	6:C:504:HOH:O	1.96	0.65
2:E:46(K)[B]:A:C2'	2:E:46(L)[B]:C:H5'	2.26	0.65
1:C:248:PRO:HA	1:C:274:ARG:HH21	1.62	0.65
2:E:10[B]:C:O2'	2:E:11[B]:C:H6	1.79	0.64
1:A:393:SER:O	1:A:397:THR:HG23	1.96	0.64
1:B:144:THR:HB	3:B:1001:PLR:H5A2	1.79	0.64
1:C:101:ILE:O	1:C:101:ILE:HG13	1.97	0.64
2:E:46(C)[B]:G:C2'	2:E:46(D)[B]:U:C5'	2.70	0.64
2:E:46(H)[A]:G:H2'	2:E:46(I)[A]:C:H6	1.63	0.64
2:E:14[A]:A:H2'	2:E:15[A]:G:C8	2.33	0.64
2:E:14[B]:A:H2'	2:E:15[B]:G:C8	2.33	0.64
2:E:46(H)[B]:G:H2'	2:E:46(I)[B]:C:H6	1.63	0.64
1:D:144:THR:HB	3:D:1001:PLR:H5A2	1.79	0.64
2:E:46(H)[B]:G:H2'	2:E:46(I)[B]:C:C6	2.33	0.64
1:D:429:TYR:CG	1:D:430:PRO:HD2	2.33	0.64
2:E:10[A]:C:O2'	2:E:11[A]:C:H6	1.79	0.64
1:B:348:LEU:O	1:B:352:ILE:HG12	1.98	0.63
2:E:64[A]:C:H2'	2:E:65[A]:C:C6	2.33	0.63
1:B:253:ASN:HD22	1:B:280:GLN:HG2	1.62	0.63
1:C:108:ALA:HB1	1:C:111:SER:HB2	1.79	0.63
1:C:144:THR:HB	3:C:1001:PLR:H5A2	1.79	0.63
1:A:278:PHE:HD2	1:A:280:GLN:HE21	1.47	0.63
2:E:46(H)[A]:G:H2'	2:E:46(I)[A]:C:C6	2.33	0.63
1:C:141:PRO:HG2	1:C:314:ALA:HB1	1.81	0.63
2:E:64[B]:C:H2'	2:E:65[B]:C:H6	1.64	0.63
2:E:11[A]:C:H2'	2:E:12[A]:U:C6	2.34	0.62
2:E:64[B]:C:H2'	2:E:65[B]:C:C6	2.33	0.62
1:D:348:LEU:O	1:D:352:ILE:HG13	1.98	0.62
2:E:11[B]:C:H2'	2:E:12[B]:U:C6	2.34	0.62
1:D:97:ARG:HB3	5:D:2001[A]:SEP:H	1.65	0.62
1:D:172:GLN:NE2	1:D:174:SER:HB3	2.14	0.62
1:A:248:PRO:HA	1:A:276:ASP:OD2	2.00	0.62
1:C:336:LYS:HE2	1:C:340:GLU:OE2	1.99	0.61
1:D:429:TYR:CD1	1:D:430:PRO:HD2	2.34	0.61
1:D:361:GLU:OE2	1:D:379:THR:HG23	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:GLN:HE21	1:B:174:SER:HB3	1.62	0.61
2:E:10[B]:C:C4	2:E:44[B]:A:N6	2.69	0.61
2:E:64[A]:C:H2'	2:E:65[A]:C:H6	1.64	0.61
2:E:10[A]:C:C4	2:E:44[A]:A:N6	2.69	0.61
1:C:313:ARG:HD3	6:C:523:HOH:O	2.01	0.61
2:E:14[B]:A:H2'	2:E:15[B]:G:H8	1.65	0.61
1:B:390:GLN:O	1:B:394:MET:HG3	2.01	0.61
2:E:46(C)[A]:G:C2'	2:E:46(D)[A]:U:C5'	2.70	0.61
1:A:33:ARG:HH22	2:E:42[B]:G:P	2.23	0.61
2:E:20(A)[A]:C:O2'	2:E:21[A]:U:C6	2.54	0.61
2:E:46(E)[B]:C:C2'	2:E:46(F)[B]:U:H5'	2.30	0.60
1:A:429:TYR:CG	1:A:430:PRO:HD2	2.36	0.60
1:C:278:PHE:CD2	1:C:280:GLN:NE2	2.69	0.60
1:C:422:PHE:O	1:C:423:MET:HB2	2.01	0.60
2:E:46(E)[A]:C:C2'	2:E:46(F)[A]:U:H5'	2.30	0.60
1:B:429:TYR:CG	1:B:430:PRO:HD2	2.37	0.60
2:E:42[A]:G:H2'	2:E:43[A]:U:C6	2.36	0.60
1:A:131:VAL:HG23	1:A:263:MET:HE3	1.84	0.60
1:C:63:SER:HA	1:C:66:PHE:CD2	2.37	0.60
1:B:122:VAL:HG13	1:B:294:ILE:HD13	1.83	0.60
1:B:100:ASP:C	1:B:102:SER:H	2.09	0.60
1:B:413:THR:OG1	1:B:418:THR:HG22	2.01	0.59
2:E:42[B]:G:H2'	2:E:43[B]:U:C6	2.37	0.59
1:D:166:ILE:HB	1:D:220:ILE:HD13	1.85	0.59
1:D:317:SER:HB3	1:D:318:PRO:HD3	1.84	0.59
1:B:449:LEU:O	1:B:453:ARG:HG3	2.02	0.59
2:E:14[A]:A:H2'	2:E:15[A]:G:H8	1.65	0.58
1:B:97:ARG:HB3	5:B:2001[A]:SEP:H	1.68	0.58
2:E:10[B]:C:H6	2:E:10[B]:C:H5'	1.68	0.58
1:D:75:ARG:HH11	5:D:2001[B]:SEP:HB2	1.69	0.58
1:A:36:LEU:CD2	1:A:117:ILE:HD11	2.34	0.58
1:B:449:LEU:HD22	1:B:453:ARG:NH1	2.17	0.58
1:A:156:ARG:HB2	1:A:184:PHE:HZ	1.68	0.58
1:A:63:SER:HA	1:A:66:PHE:CD2	2.38	0.58
1:C:429:TYR:CG	1:C:430:PRO:HD2	2.39	0.58
2:E:67(A)[B]:U:H2'	2:E:67(B)[B]:U:C6	2.39	0.57
2:E:10[A]:C:H6	2:E:10[A]:C:H5'	1.68	0.57
1:D:122:VAL:HG13	1:D:294:ILE:HD13	1.85	0.57
1:B:122:VAL:CG1	1:B:294:ILE:HD13	2.34	0.57
1:C:100:ASP:HB3	1:C:103:ALA:HB2	1.85	0.57
2:E:41[B]:U:H2'	2:E:42[B]:G:H8	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ARG:NH2	2:E:42[B]:G:OP1	2.29	0.57
1:C:257:VAL:CG2	1:C:280:GLN:HG2	2.34	0.57
2:E:46(J)[A]:G:H2'	2:E:46(K)[A]:A:H8	1.69	0.57
1:B:382:GLU:HA	1:B:386:LYS:HA	1.86	0.57
2:E:20(A)[B]:C:HO2'	2:E:21[B]:U:H6	1.43	0.57
2:E:47[A]:A:H2'	2:E:48[A]:G:H8	1.71	0.56
2:E:67(A)[A]:U:H2'	2:E:67(B)[A]:U:C6	2.39	0.56
1:C:105:GLN:HG3	1:C:107:LYS:H	1.69	0.56
1:B:398:ARG:HG2	1:B:456:ARG:HH21	1.70	0.56
2:E:59[B]:U:O2'	2:E:60[B]:U:C5'	2.53	0.56
1:C:282:LEU:HD22	1:C:322:VAL:HG11	1.86	0.56
2:E:41[A]:U:H2'	2:E:42[A]:G:H8	1.69	0.56
2:E:59[A]:U:O2'	2:E:60[A]:U:C5'	2.53	0.56
2:E:66[A]:U:H2'	2:E:67(A)[A]:U:O4'	2.06	0.56
1:B:43[B]:GLU:HG2	1:B:332:ASN:ND2	2.21	0.56
1:A:390:GLN:O	1:A:394:MET:HG3	2.05	0.55
1:C:86:ARG:HH12	1:D:86:ARG:CZ	2.18	0.55
1:D:96:GLY:HA3	1:D:101:ILE:HA	1.88	0.55
2:E:66[B]:U:H2'	2:E:67(A)[B]:U:O4'	2.06	0.55
2:E:46(F)[B]:U:O2'	2:E:46(H)[B]:G:N7	2.37	0.55
1:B:192:VAL:HG23	1:B:201:ASP:HB2	1.88	0.55
1:C:154:THR:HA	1:C:309:MET:HE3	1.87	0.55
1:A:404:ARG:HB3	1:A:435:ASN:HB2	1.88	0.55
1:C:393:SER:O	1:C:397:THR:HG23	2.06	0.55
1:B:443:LYS:O	1:B:446:ASP:HB2	2.07	0.55
1:C:172:GLN:NE2	1:C:174:SER:HB3	2.22	0.55
2:E:10[B]:C:O2'	2:E:11[B]:C:C6	2.60	0.55
1:B:198:LEU:CD2	1:B:426:THR:HG21	2.37	0.55
1:B:202:LEU:HD11	1:B:234:ARG:HD2	1.89	0.55
1:D:399:GLN:HG3	2:E:1[B]:G:O4'	2.07	0.54
1:A:24:ALA:C	1:A:26:ARG:H	2.14	0.54
1:B:197:GLU:CD	1:B:368:HIS:HD1	2.16	0.54
1:A:365:HIS:C	1:A:367:PRO:HD3	2.32	0.54
1:D:122:VAL:CG1	1:D:294:ILE:HD13	2.38	0.54
2:E:11[A]:C:H2'	2:E:12[A]:U:H6	1.73	0.54
1:A:105:GLN:OE1	1:A:106:PRO:HD2	2.07	0.54
2:E:15[B]:G:H2'	2:E:16[B]:U:O5'	2.07	0.54
2:E:45[B]:G:H2'	2:E:46(A)[B]:C:C5'	2.38	0.54
2:E:46(B)[A]:U:H6	2:E:46(B)[A]:U:O5'	1.91	0.54
1:D:437:ALA:O	1:D:442:MET:HE1	2.06	0.54
2:E:15[A]:G:H2'	2:E:16[A]:U:O5'	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:43[B]:U:O5'	2:E:43[B]:U:H6	1.91	0.54
1:B:229:PRO:HD3	1:B:433:TYR:CZ	2.43	0.54
1:B:281:SER:OG	1:B:283:ASP:OD1	2.25	0.54
1:B:359:TYR:CE1	1:B:458:LEU:HB3	2.43	0.54
2:E:70[B]:G:H2'	2:E:71[B]:G:C8	2.43	0.54
1:A:356:SER:OG	1:A:362:ARG:HA	2.08	0.53
2:E:13[B]:C:N3	2:E:22[B]:G:O6	2.41	0.53
1:B:105:GLN:NE2	1:B:313:ARG:HH21	2.06	0.53
1:C:172:GLN:HG2	3:C:1001:PLR:N1	2.23	0.53
2:E:10[A]:C:O2'	2:E:11[A]:C:C6	2.60	0.53
2:E:46(B)[B]:U:O5'	2:E:46(B)[B]:U:H6	1.91	0.53
1:C:255:TYR:HB3	1:C:284:LYS:HB3	1.90	0.53
2:E:13[A]:C:N3	2:E:22[A]:G:O6	2.41	0.53
2:E:43[A]:U:O5'	2:E:43[A]:U:H6	1.91	0.53
2:E:46(J)[B]:G:H2'	2:E:46(K)[B]:A:H8	1.69	0.53
2:E:11[B]:C:H2'	2:E:12[B]:U:H6	1.73	0.53
2:E:70[A]:G:H2'	2:E:71[A]:G:C8	2.43	0.53
1:C:220:ILE:HD12	1:C:242:CYS:SG	2.49	0.53
1:D:185:GLU:HG3	1:D:417[B]:TYR:OH	2.09	0.53
2:E:8[B]:A:H1'	2:E:49[B]:A:N3	2.24	0.53
1:D:75:ARG:NH1	5:D:2001[B]:SEP:HB2	2.24	0.53
1:D:382:GLU:HA	1:D:386:LYS:HA	1.89	0.53
2:E:10[A]:C:N3	2:E:44[A]:A:N6	2.57	0.53
2:E:46(B)[A]:U:O2'	2:E:46(C)[A]:G:H5'	2.09	0.53
1:B:422:PHE:O	1:B:423:MET:HB2	2.09	0.52
1:A:69:ASN:HB3	6:A:514:HOH:O	2.08	0.52
1:B:282:LEU:HD12	1:B:292:GLY:HA3	1.91	0.52
1:C:452:LYS:HE2	1:C:456:ARG:NH2	2.23	0.52
2:E:10[B]:C:N3	2:E:44[B]:A:N6	2.57	0.52
1:A:257:VAL:HB	1:A:285:ASN:ND2	2.25	0.52
2:E:45[A]:G:H2'	2:E:46(A)[A]:C:C5'	2.38	0.52
1:A:429:TYR:CD1	1:A:430:PRO:HD2	2.44	0.52
2:E:8[A]:A:H1'	2:E:49[A]:A:N3	2.24	0.52
1:A:336:LYS:HE2	1:A:340:GLU:OE2	2.09	0.52
1:D:114:LEU:C	1:D:114:LEU:HD23	2.35	0.52
1:B:425:HIS:O	1:B:426:THR:HG23	2.09	0.52
1:C:255:TYR:HA	1:C:285:ASN:HD21	1.74	0.52
1:B:132:HIS:H	1:B:267:GLN:NE2	2.07	0.52
1:C:131:VAL:HG23	1:C:263:MET:HE3	1.91	0.52
1:C:248:PRO:N	1:C:274:ARG:HH21	2.07	0.52
1:D:287:MET:HE1	1:D:337:LEU:CD1	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:29[A]:A:C4	2:E:42[A]:G:N2	2.78	0.52
1:C:297:GLY:HA3	1:C:303:ILE:HD11	1.92	0.52
2:E:46(B)[B]:U:O2'	2:E:46(C)[B]:G:H5'	2.09	0.52
2:E:46(F)[A]:U:O2'	2:E:46(H)[A]:G:N7	2.37	0.52
2:E:49[A]:A:C3'	2:E:50[A]:G:H5'	2.39	0.51
1:A:255:TYR:HB3	1:A:284:LYS:HB3	1.91	0.51
1:A:144:THR:OG1	1:A:281:SER:HB2	2.10	0.51
1:B:105:GLN:OE1	1:B:106:PRO:HD2	2.09	0.51
1:C:114:LEU:C	1:C:114:LEU:HD23	2.35	0.51
2:E:29[B]:A:C4	2:E:42[B]:G:N2	2.78	0.51
2:E:46(C)[A]:G:C6	2:E:47[A]:A:N1	2.79	0.51
1:A:141:PRO:HG2	1:A:314:ALA:CB	2.41	0.51
1:B:344:MET:HE1	1:B:444:MET:HA	1.91	0.51
2:E:31[A]:G:O5'	2:E:31[A]:G:H8	1.94	0.51
1:C:172:GLN:HE21	1:C:174:SER:N	2.07	0.51
2:E:46(C)[B]:G:C6	2:E:47[B]:A:N1	2.79	0.51
2:E:47[B]:A:H2'	2:E:48[B]:G:H8	1.71	0.51
2:E:46(H)[A]:G:HO2'	2:E:46(I)[A]:C:H5'	1.74	0.51
1:B:255:TYR:HB3	1:B:284:LYS:HD3	1.92	0.50
1:C:382:GLU:OE2	1:C:389:THR:HG23	2.11	0.50
1:D:128:LEU:CD1	1:D:335:LYS:HE3	2.28	0.50
1:B:297:GLY:CA	1:B:303:ILE:HD11	2.36	0.50
1:C:69:ASN:HB3	6:C:518:HOH:O	2.10	0.50
2:E:49[B]:A:C3'	2:E:50[B]:G:H5'	2.39	0.50
1:A:121:LEU:HD12	1:A:323:LEU:HD12	1.94	0.50
1:B:457:CYS:O	1:B:461:VAL:HG23	2.11	0.50
1:D:97:ARG:CB	5:D:2001[A]:SEP:H	2.23	0.50
1:D:443:LYS:O	1:D:446:ASP:HB2	2.12	0.50
2:E:14[A]:A:H1'	2:E:22[A]:G:N2	2.27	0.50
2:E:31[B]:G:O5'	2:E:31[B]:G:H8	1.94	0.50
1:D:229:PRO:HD3	1:D:433:TYR:CZ	2.46	0.50
2:E:69[B]:G:H2'	2:E:70[B]:G:H8	1.77	0.49
1:A:284:LYS:NZ	3:A:1001:PLR:O3	2.45	0.49
1:A:234:ARG:HB3	1:A:237:GLU:OE1	2.12	0.49
1:A:220:ILE:HD12	1:A:242:CYS:SG	2.52	0.49
1:B:101:ILE:HG22	1:B:307:SER:O	2.13	0.49
1:B:202:LEU:HD13	1:B:237:GLU:HG2	1.94	0.49
1:B:400:VAL:HG22	1:B:453:ARG:HD2	1.93	0.49
2:E:10[B]:C:H5'	2:E:10[B]:C:C6	2.47	0.49
2:E:14[B]:A:H1'	2:E:22[B]:G:N2	2.27	0.49
2:E:58[B]:A:O2'	2:E:59[B]:U:H3'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:422:PHE:O	1:D:423:MET:HB2	2.13	0.49
2:E:45[B]:G:O5'	2:E:45[B]:G:H8	1.96	0.49
2:E:10[A]:C:H5'	2:E:10[A]:C:C6	2.47	0.49
1:A:128:LEU:HD23	1:A:128:LEU:C	2.37	0.49
1:A:278:PHE:CE2	1:A:280:GLN:NE2	2.80	0.49
1:C:172:GLN:NE2	1:C:174:SER:H	2.07	0.49
2:E:58[A]:A:O2'	2:E:59[A]:U:H3'	2.12	0.49
1:C:122:VAL:CG1	1:C:294:ILE:HD13	2.43	0.49
1:C:457:CYS:O	1:C:461:VAL:HG23	2.13	0.49
2:E:45[A]:G:O5'	2:E:45[A]:G:H8	1.96	0.49
2:E:69[A]:G:H2'	2:E:70[A]:G:H8	1.77	0.49
1:A:154:THR:HA	1:A:309:MET:HE3	1.94	0.48
2:E:27[B]:G:C2	2:E:44[B]:A:C4	3.01	0.48
1:A:33:ARG:NH2	2:E:41[B]:U:O3'	2.47	0.48
2:E:27[A]:G:C2	2:E:44[A]:A:C4	3.01	0.48
1:A:394:MET:HE1	1:A:460:ALA:HB3	1.95	0.48
1:A:24:ALA:C	1:A:26:ARG:N	2.72	0.48
1:A:206:GLU:O	1:A:209:VAL:HG12	2.12	0.48
1:B:449:LEU:HD22	1:B:453:ARG:HH11	1.78	0.48
1:C:248:PRO:HA	1:C:276:ASP:OD2	2.14	0.48
1:C:394:MET:HE1	1:C:460:ALA:HB3	1.96	0.48
1:C:268:GLN:HE22	1:C:271:ARG:NE	2.12	0.48
2:E:20(A)[A]:C:C5	2:E:59[A]:U:C4	3.02	0.48
1:B:359:TYR:OH	1:B:459:LYS:HG3	2.14	0.48
1:A:258:GLN:HA	1:A:338:LEU:HD21	1.96	0.47
1:C:390:GLN:O	1:C:394:MET:HG3	2.13	0.47
2:E:20(A)[B]:C:C5	2:E:59[B]:U:C4	3.02	0.47
1:B:425:HIS:O	1:B:426:THR:CG2	2.61	0.47
1:D:449:LEU:O	1:D:453:ARG:HG3	2.14	0.47
2:E:46(C)[B]:G:H2'	2:E:46(D)[B]:U:C5'	2.37	0.47
1:B:43[B]:GLU:HG2	1:B:332:ASN:HD21	1.79	0.47
1:A:366:THR:N	1:A:367:PRO:HD3	2.29	0.47
1:B:75:ARG:HD3	1:B:313:ARG:NH1	2.29	0.47
1:C:26:ARG:HD2	2:E:2[B]:C:O3'	2.15	0.47
1:D:169:ARG:NH1	1:D:427:ASN:OD1	2.45	0.47
2:E:15[A]:G:C2'	2:E:16[A]:U:O5'	2.62	0.47
1:B:425:HIS:C	1:B:426:THR:HG23	2.40	0.47
1:D:417[A]:TYR:HD2	1:D:419:PHE:CE2	2.33	0.47
1:D:202:LEU:CD1	1:D:237:GLU:HG2	2.44	0.47
2:E:14[A]:A:C4	2:E:22[A]:G:N1	2.83	0.47
2:E:15[B]:G:C2'	2:E:16[B]:U:O5'	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:20(A)[B]:C:O2'	2:E:21[B]:U:C6	2.54	0.47
1:A:172:GLN:NE2	1:A:174:SER:HB3	2.27	0.47
1:C:172:GLN:O	1:C:172:GLN:HG3	2.14	0.47
2:E:27[A]:G:H2'	2:E:28[A]:C:H6	1.80	0.47
1:A:118:THR:HG23	1:A:322:VAL:HG12	1.95	0.47
1:C:365:HIS:C	1:C:367:PRO:HD3	2.40	0.47
1:C:278:PHE:HD2	1:C:280:GLN:NE2	2.11	0.46
1:C:345:PHE:CZ	1:C:373:LEU:HD21	2.51	0.46
1:D:184:PHE:CE2	1:D:218:LEU:HD22	2.50	0.46
2:E:24[B]:G:H2'	2:E:25[B]:G:H8	1.80	0.46
1:A:310:TYR:HA	1:A:311:PRO:HD3	1.65	0.46
1:B:248:PRO:HA	1:B:276:ASP:OD2	2.15	0.46
2:E:11[B]:C:C2	2:E:12[B]:U:C5	3.03	0.46
1:C:105:GLN:HG3	1:C:107:LYS:N	2.30	0.46
2:E:14[B]:A:C4	2:E:15[B]:G:C8	3.03	0.46
1:B:356:SER:HB3	1:B:361:GLU:O	2.15	0.46
1:C:228:ALA:H	1:C:372:SER:HB3	1.81	0.46
1:C:429:TYR:CD1	1:C:430:PRO:HD2	2.50	0.46
1:D:445:GLN:O	1:D:449:LEU:HD13	2.15	0.46
1:B:391:LEU:O	1:B:391:LEU:HG	2.15	0.46
1:C:128:LEU:HD12	1:C:128:LEU:O	2.16	0.46
2:E:39[A]:C:H2'	2:E:40[A]:C:C6	2.45	0.46
2:E:49[A]:A:C4'	2:E:50[A]:G:C5'	2.75	0.46
1:A:100:ASP:OD1	1:A:308:LYS:HG2	2.14	0.46
1:A:253:ASN:HD22	1:A:280:GLN:HG3	1.78	0.46
1:C:172:GLN:HE21	1:C:174:SER:HB3	1.81	0.46
1:C:173:LYS:O	1:C:177:LYS:HG3	2.16	0.46
2:E:27[B]:G:H2'	2:E:28[B]:C:H6	1.80	0.46
2:E:52[A]:G:O2'	2:E:53[A]:G:H5'	2.16	0.46
2:E:14[A]:A:C4	2:E:15[A]:G:C8	3.03	0.46
2:E:24[A]:G:H2'	2:E:25[A]:G:H8	1.80	0.46
1:C:30:HIS:CD2	2:E:41[A]:U:H5''	2.51	0.46
1:D:202:LEU:HD13	1:D:237:GLU:HG2	1.98	0.46
2:E:46(J)[B]:G:O5'	2:E:46(J)[B]:G:H8	1.99	0.46
1:A:155:LEU:HD11	1:A:250:ILE:CD1	2.45	0.46
1:B:397:THR:HG21	2:E:73[A]:G:H1'	1.97	0.46
1:C:140:VAL:HA	1:C:141:PRO:HD3	1.84	0.46
1:D:253:ASN:HB3	1:D:280:GLN:HG3	1.98	0.46
2:E:14[B]:A:C4	2:E:22[B]:G:N1	2.83	0.46
2:E:27[A]:G:H2'	2:E:28[A]:C:C6	2.51	0.46
2:E:27[B]:G:H2'	2:E:28[B]:C:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:43[A]:U:C6	2:E:43[A]:U:O5'	2.69	0.46
2:E:11[A]:C:C2	2:E:12[A]:U:C5	3.03	0.46
1:B:355:LEU:HD12	1:B:355:LEU:O	2.16	0.45
2:E:46(A)[A]:C:H3'	2:E:46(B)[A]:U:C5	2.51	0.45
2:E:52[B]:G:O2'	2:E:53[B]:G:H5'	2.16	0.45
1:D:399:GLN:CG	2:E:1[B]:G:O4'	2.64	0.45
1:A:100:ASP:C	1:A:102:SER:H	2.23	0.45
1:B:395:LEU:O	1:B:400:VAL:HG23	2.17	0.45
1:C:144:THR:OG1	1:C:281:SER:HB3	2.15	0.45
1:C:317:SER:HB3	1:C:318:PRO:HD3	1.98	0.45
1:A:100:ASP:HB2	1:A:103:ALA:HB2	1.96	0.45
1:A:155:LEU:HD11	1:A:250:ILE:HD11	1.98	0.45
1:A:259:SER:HB2	1:A:371:ILE:HD11	1.99	0.45
1:C:100:ASP:C	1:C:102:SER:H	2.25	0.45
1:D:128:LEU:CD1	1:D:335:LYS:HE2	2.32	0.45
1:D:355:LEU:C	1:D:355:LEU:HD23	2.42	0.45
1:D:376:THR:O	1:D:377:LEU:HD23	2.16	0.45
2:E:46(A)[B]:C:H3'	2:E:46(B)[B]:U:C5	2.51	0.45
1:A:297:GLY:HA3	1:A:303:ILE:HD11	1.98	0.45
1:B:378:LYS:HB3	1:B:378:LYS:HE2	1.77	0.45
1:C:86:ARG:NH1	1:D:86:ARG:CZ	2.79	0.45
2:E:46(J)[A]:G:O5'	2:E:46(J)[A]:G:H8	1.99	0.45
1:B:51:LEU:HD21	1:B:324:ILE:HG23	1.98	0.45
1:C:58:LEU:O	1:C:61:MET:HB2	2.17	0.45
1:C:233:ASP:HA	6:C:528:HOH:O	2.16	0.45
2:E:1[A]:G:H2'	2:E:2[A]:C:C6	2.51	0.45
2:E:50[B]:G:N3	2:E:50[B]:G:H2'	2.32	0.45
2:E:67(A)[B]:U:H2'	2:E:67(B)[B]:U:H6	1.81	0.45
1:C:348:LEU:HG	1:C:373:LEU:HD12	1.98	0.45
2:E:1[B]:G:H2'	2:E:2[B]:C:C6	2.51	0.45
2:E:67(A)[A]:U:H2'	2:E:67(B)[A]:U:H6	1.82	0.45
1:C:26:ARG:HA	1:C:29[A]:GLU:OE1	2.17	0.45
2:E:11[B]:C:C4	2:E:25[B]:G:N1	2.85	0.45
1:B:125:ILE:HD13	1:B:128:LEU:HD23	1.99	0.45
2:E:52[A]:G:C2'	2:E:53[A]:G:H5'	2.47	0.45
2:E:52[B]:G:C2'	2:E:53[B]:G:H5'	2.47	0.45
1:A:97:ARG:HG2	1:A:105:GLN:HB2	1.99	0.44
1:B:194:GLU:OE2	1:B:234:ARG:NH2	2.50	0.44
1:C:336:LYS:O	1:C:340:GLU:HG3	2.16	0.44
2:E:11[A]:C:C4	2:E:25[A]:G:N1	2.85	0.44
2:E:25[B]:G:H2'	2:E:26[B]:U:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:VAL:HG12	1:B:194:GLU:HG3	1.99	0.44
1:D:397:THR:HG21	2:E:73[B]:G:H1'	1.97	0.44
2:E:46(C)[A]:G:H2'	2:E:46(D)[A]:U:C5'	2.37	0.44
1:A:219:CYS:HB2	1:A:248:PRO:O	2.17	0.44
1:B:41:CYS:HA	1:B:121:LEU:HD22	1.99	0.44
1:B:128:LEU:O	1:B:128:LEU:HD12	2.17	0.44
2:E:50[A]:G:N3	2:E:50[A]:G:H2'	2.32	0.44
1:A:422:PHE:O	1:A:423:MET:CB	2.60	0.44
1:A:443:LYS:O	1:A:446:ASP:HB2	2.17	0.44
1:B:141:PRO:HG2	1:B:314:ALA:CB	2.41	0.44
2:E:49[B]:A:C4'	2:E:50[B]:G:C5'	2.75	0.44
1:B:326:LEU:HD23	1:B:326:LEU:HA	1.79	0.44
2:E:43[B]:U:C6	2:E:43[B]:U:O5'	2.69	0.44
1:A:114:LEU:C	1:A:114:LEU:HD23	2.42	0.44
1:C:422:PHE:O	1:C:423:MET:CB	2.63	0.44
2:E:29[A]:A:C2	2:E:42[A]:G:C2	3.05	0.44
1:B:114:LEU:HD23	1:B:114:LEU:C	2.43	0.44
1:C:310:TYR:HA	1:C:311:PRO:HD3	1.67	0.44
1:D:192:VAL:HG23	1:D:201:ASP:HB2	2.00	0.44
1:B:62:ASP:HB3	1:B:64:ASN:OD1	2.18	0.44
1:C:100:ASP:HB3	1:C:103:ALA:CB	2.47	0.44
2:E:25[A]:G:H2'	2:E:26[A]:U:C6	2.52	0.44
2:E:70[B]:G:H2'	2:E:71[B]:G:H8	1.83	0.44
1:B:411:MET:HE2	1:B:411:MET:HB3	1.83	0.44
1:C:261:LYS:HG2	1:C:370:PRO:HG3	1.98	0.44
1:C:140:VAL:HG21	1:C:142:MET:HE2	2.00	0.43
2:E:29[B]:A:C2	2:E:42[B]:G:C2	3.06	0.43
1:C:41:CYS:SG	1:C:125:ILE:HD13	2.58	0.43
1:C:189:ILE:HD11	1:C:208:LYS:HG3	2.00	0.43
1:A:317:SER:HB3	1:A:318:PRO:HD3	1.99	0.43
1:D:242:CYS:HB3	1:D:247:ILE:O	2.18	0.43
1:B:253:ASN:ND2	1:B:280:GLN:HG2	2.31	0.43
1:B:278:PHE:CE2	1:B:280:GLN:NE2	2.85	0.43
2:E:27[A]:G:N1	2:E:44[A]:A:C5	2.87	0.43
2:E:27[B]:G:N1	2:E:44[B]:A:C5	2.87	0.43
2:E:46(H)[B]:G:C2'	2:E:46(I)[B]:C:C5'	2.94	0.43
1:A:394:MET:HE2	1:A:394:MET:HB3	1.85	0.43
1:C:51:LEU:HD21	1:C:324:ILE:HG23	2.00	0.43
1:C:101:ILE:HG22	1:C:307:SER:O	2.18	0.43
1:C:105:GLN:CG	1:C:107:LYS:HB2	2.48	0.43
2:E:39[B]:C:H2'	2:E:40[B]:C:C6	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:2002:SEP:O1P	5:B:2002:SEP:HA	2.19	0.43
1:A:206:GLU:HA	1:A:209:VAL:HG12	2.00	0.43
1:B:429:TYR:CD1	1:B:430:PRO:HD2	2.53	0.43
1:D:141:PRO:HG2	1:D:314:ALA:CB	2.40	0.43
1:D:75:ARG:HD2	5:D:2001[B]:SEP:HB2	2.00	0.43
1:D:252:ASN:OD1	1:D:252:ASN:C	2.61	0.43
1:D:390:GLN:O	1:D:394:MET:HG3	2.18	0.43
1:D:359:TYR:CE1	1:D:458:LEU:HB3	2.54	0.43
2:E:42[A]:G:H2'	2:E:43[A]:U:H6	1.82	0.43
1:A:189:ILE:HD11	1:A:208:LYS:HG3	1.99	0.43
1:C:394:MET:HE2	1:C:394:MET:HB3	1.80	0.43
2:E:13[A]:C:C2	2:E:14[A]:A:C8	3.07	0.43
1:A:224:THR:CG2	1:A:235:LEU:HD11	2.49	0.42
1:B:310:TYR:HA	1:B:311:PRO:HD3	1.79	0.42
2:E:46(A)[A]:C:C2'	2:E:46(B)[A]:U:C6	2.98	0.42
2:E:30[B]:G:N2	2:E:40[B]:C:O2	2.50	0.42
1:C:449:LEU:HD23	1:C:449:LEU:HA	1.90	0.42
1:D:51:LEU:HD21	1:D:324:ILE:HG23	2.02	0.42
2:E:20(A)[A]:C:N4	2:E:59[A]:U:C2	2.87	0.42
1:B:43[B]:GLU:CD	1:B:332:ASN:HD21	2.27	0.42
1:B:132:HIS:H	1:B:267:GLN:HE21	1.66	0.42
2:E:46(D)[A]:U:H2'	2:E:46(E)[A]:C:C6	2.54	0.42
1:A:33:ARG:NH2	2:E:42[B]:G:P	2.91	0.42
1:B:340:GLU:O	1:B:344:MET:HG2	2.19	0.42
1:B:369:ASN:HA	1:B:370:PRO:HD3	1.81	0.42
1:D:140:VAL:HA	1:D:141:PRO:HD3	1.76	0.42
2:E:29[B]:A:C6	2:E:42[B]:G:N1	2.88	0.42
1:B:271:ARG:HD2	6:B:506:HOH:O	2.18	0.42
2:E:20(A)[B]:C:N4	2:E:59[B]:U:C2	2.87	0.42
1:A:185:GLU:HA	1:A:186:PRO:HD3	1.84	0.42
1:C:45:GLY:HA3	1:C:328:SER:O	2.19	0.42
1:C:128:LEU:HD12	1:C:128:LEU:C	2.45	0.42
1:D:229:PRO:HD3	1:D:433:TYR:CE1	2.55	0.42
1:A:122:VAL:CG1	1:A:294:ILE:HD13	2.50	0.42
1:A:185:GLU:HG3	1:A:417[A]:TYR:OH	2.20	0.42
1:B:220:ILE:HD12	1:B:242:CYS:SG	2.60	0.42
1:B:359:TYR:O	1:B:360:ASN:HB2	2.18	0.42
1:C:158:LYS:HD3	1:C:305:GLU:OE1	2.20	0.42
1:D:97:ARG:HG2	1:D:105:GLN:NE2	2.33	0.42
1:D:100:ASP:C	1:D:102:SER:H	2.28	0.42
1:D:257:VAL:HG23	1:D:280:GLN:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:46(D)[B]:U:H2'	2:E:46(E)[B]:C:C6	2.54	0.42
1:A:445:GLN:HE21	1:A:449:LEU:CD1	2.32	0.42
1:B:393:SER:HB2	2:E:73[A]:G:O2'	2.19	0.42
1:C:185:GLU:HA	1:C:186:PRO:HD3	1.90	0.42
1:C:236:GLU:H	1:C:236:GLU:HG2	1.53	0.42
1:C:366:THR:N	1:C:367:PRO:HD3	2.35	0.42
2:E:29[A]:A:C6	2:E:42[A]:G:N1	2.88	0.42
1:B:97:ARG:CB	5:B:2001[A]:SEP:H	2.32	0.42
1:D:231:VAL:HB	1:D:232:PRO:HD2	2.01	0.42
1:D:336:LYS:HE2	1:D:340:GLU:OE2	2.20	0.42
2:E:13[B]:C:C2	2:E:14[B]:A:C8	3.07	0.42
2:E:24[B]:G:H2'	2:E:25[B]:G:C8	2.54	0.42
2:E:61[A]:C:HO2'	2:E:62[A]:C:H6	1.64	0.42
1:A:253:ASN:ND2	1:A:280:GLN:HG2	2.31	0.41
1:C:98:SER:HA	1:C:312:GLY:HA2	2.02	0.41
1:C:394:MET:HE1	1:C:460:ALA:CB	2.50	0.41
1:B:184:PHE:CZ	1:B:218:LEU:HD13	2.55	0.41
1:C:219:CYS:HB2	1:C:248:PRO:O	2.20	0.41
1:D:148:LEU:HD23	1:D:279:VAL:HG21	2.02	0.41
2:E:46(E)[B]:C:C3'	2:E:46(F)[B]:U:H5'	2.50	0.41
2:E:52[B]:G:C2	2:E:63[B]:A:C2	3.09	0.41
1:A:101:ILE:HG12	1:A:101:ILE:O	2.20	0.41
1:A:149:THR:HG23	1:A:182:ALA:HB2	2.03	0.41
1:A:271:ARG:NH1	2:E:56[B]:C:OP1	2.52	0.41
1:B:100:ASP:C	1:B:102:SER:N	2.74	0.41
1:B:100:ASP:HB3	1:B:102:SER:HB2	2.02	0.41
1:C:177:LYS:O	1:C:178:SER:C	2.63	0.41
1:C:443:LYS:O	1:C:446:ASP:HB2	2.20	0.41
1:D:63:SER:HA	1:D:66:PHE:CD2	2.56	0.41
2:E:24[A]:G:H2'	2:E:25[A]:G:C8	2.54	0.41
2:E:46(E)[A]:C:C3'	2:E:46(F)[A]:U:H5'	2.50	0.41
2:E:70[A]:G:H2'	2:E:71[A]:G:H8	1.83	0.41
1:B:222:SER:OG	1:B:251:VAL:HG22	2.20	0.41
1:B:348:LEU:HD23	1:B:373:LEU:HD12	2.03	0.41
1:D:167:TRP:CD1	1:D:221:HIS:CD2	3.08	0.41
1:D:226:CYS:SG	1:D:230:ARG:HD3	2.60	0.41
1:D:349:SER:O	1:D:350:ASN:C	2.64	0.41
2:E:5(A)[A]:G:O2'	2:E:5(B)[A]:G:H5'	2.20	0.41
2:E:46(H)[A]:G:C2'	2:E:46(I)[A]:C:C5'	2.94	0.41
2:E:59[A]:U:H2'	2:E:60[A]:U:C6	2.56	0.41
1:A:63:SER:HA	1:A:66:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ASN:HA	1:A:370:PRO:HD3	1.72	0.41
1:A:424:SER:O	1:A:425:HIS:HB2	2.21	0.41
1:B:75:ARG:HH11	5:B:2001[B]:SEP:HB2	1.85	0.41
1:B:140:VAL:HA	1:B:141:PRO:HD3	1.79	0.41
2:E:52[A]:G:C2	2:E:63[A]:A:C2	3.09	0.41
1:A:140:VAL:HA	1:A:141:PRO:HD3	1.74	0.41
1:C:284:LYS:NZ	3:C:1001:PLR:O3	2.54	0.41
1:B:202:LEU:CD1	1:B:237:GLU:HG2	2.50	0.41
1:B:208:LYS:HD2	1:B:208:LYS:HA	1.89	0.41
1:B:250:ILE:HD13	1:B:250:ILE:HA	1.93	0.41
1:C:398:ARG:HD2	1:C:457:CYS:SG	2.60	0.41
1:C:408:LEU:HD21	1:C:431:CYS:C	2.46	0.41
2:E:5(A)[B]:G:O2'	2:E:5(B)[B]:G:H5'	2.20	0.41
2:E:20(A)[A]:C:C4	2:E:59[A]:U:N3	2.89	0.41
2:E:49[B]:A:H4'	2:E:50[B]:G:H5''	1.93	0.41
2:E:54[B]:U:O2	2:E:58[B]:A:N6	2.53	0.41
2:E:59[B]:U:H2'	2:E:60[B]:U:C6	2.56	0.41
2:E:66[B]:U:C4	2:E:67(A)[B]:U:C4	3.09	0.41
1:B:313:ARG:NH2	5:B:2001[B]:SEP:O2P	2.55	0.40
1:B:382:GLU:HA	1:B:386:LYS:CA	2.50	0.40
1:A:395:LEU:HD13	1:A:403:ALA:HB1	2.03	0.40
1:D:359:TYR:OH	1:D:459:LYS:HG3	2.21	0.40
2:E:20(A)[B]:C:C4	2:E:59[B]:U:N3	2.89	0.40
1:A:125:ILE:HG21	1:A:286:PHE:HE1	1.85	0.40
1:A:236:GLU:O	1:A:240:VAL:HG23	2.21	0.40
1:A:382:GLU:O	1:A:382:GLU:HG3	2.21	0.40
1:B:290:VAL:HG12	1:B:291:GLY:N	2.35	0.40
1:B:347:TYR:O	1:B:348:LEU:C	2.64	0.40
1:C:290:VAL:CG1	1:C:291:GLY:N	2.84	0.40
1:D:355:LEU:HD12	1:D:451:ILE:HG23	2.03	0.40
2:E:66[A]:U:C4	2:E:67(A)[A]:U:C4	3.09	0.40
1:A:236:GLU:HA	1:A:269:GLY:HA2	2.04	0.40
1:C:122:VAL:HG11	1:C:294:ILE:HD13	2.04	0.40
1:D:198:LEU:HD23	1:D:198:LEU:HA	1.94	0.40
1:D:420:ARG:O	1:D:427:ASN:HA	2.21	0.40
1:D:369:ASN:HA	1:D:370:PRO:HD3	1.84	0.40
2:E:10[B]:C:C4	2:E:44[B]:A:C6	3.10	0.40
2:E:41[A]:U:C2	2:E:42[A]:G:N7	2.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	445/501 (89%)	422 (95%)	21 (5%)	2 (0%)	30	58
1	B	446/501 (89%)	420 (94%)	26 (6%)	0	100	100
1	C	446/501 (89%)	420 (94%)	25 (6%)	1 (0%)	43	71
1	D	445/501 (89%)	424 (95%)	20 (4%)	1 (0%)	43	71
All	All	1782/2004 (89%)	1686 (95%)	92 (5%)	4 (0%)	43	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	384	ARG
1	D	101	ILE
1	A	101	ILE
1	C	101	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	375/430 (87%)	368 (98%)	7 (2%)	50	79
1	B	371/430 (86%)	366 (99%)	5 (1%)	61	85
1	C	372/430 (86%)	365 (98%)	7 (2%)	50	79
1	D	369/430 (86%)	364 (99%)	5 (1%)	59	84
All	All	1487/1720 (86%)	1463 (98%)	24 (2%)	55	82

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	LEU
1	A	140	VAL
1	A	236	GLU
1	A	250	ILE
1	A	380	LEU
1	A	389	THR
1	A	405	VAL
1	B	122	VAL
1	B	128	LEU
1	B	170	ILE
1	B	400	VAL
1	B	405	VAL
1	C	125	ILE
1	C	128	LEU
1	C	231	VAL
1	C	236	GLU
1	C	250	ILE
1	C	322	VAL
1	C	405	VAL
1	D	122	VAL
1	D	172	GLN
1	D	272	VAL
1	D	352	ILE
1	D	405	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	253	ASN
1	A	299	ASN
1	A	445	GLN
1	B	93	HIS
1	B	119	ASN
1	B	172	GLN
1	B	253	ASN
1	B	267	GLN
1	B	285	ASN
1	B	304	GLN
1	B	332	ASN
1	B	350	ASN
1	C	30	HIS

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Mol	Chain	Res	Type
1	C	105	GLN
1	C	132	HIS
1	C	172	GLN
1	C	268	GLN
1	C	280	GLN
1	C	285	ASN
1	C	360	ASN
1	C	365	HIS
1	C	427	ASN
1	D	88	HIS
1	D	221	HIS
1	D	285	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	0/90	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 ligands are 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	PLR	D	1001	1	15,15,15	1.05	1 (6%)	21,22,22	1.08	1 (4%)
4	TS6	A	3002	-	3,4,4	2.13	3 (100%)	3,6,6	1.24	0
5	SEP	D	2002	-	9,10,10	1.70	2 (22%)	9,14,14	1.63	2 (22%)
5	SEP	D	2001[B]	-	9,10,10	1.66	2 (22%)	9,14,14	1.55	2 (22%)
5	SEP	B	2001[A]	-	9,10,10	1.67	2 (22%)	9,14,14	1.72	2 (22%)
5	SEP	B	2001[B]	-	9,10,10	1.65	2 (22%)	9,14,14	1.53	2 (22%)
5	SEP	B	2002	-	9,10,10	1.71	2 (22%)	9,14,14	1.92	2 (22%)
4	TS6	C	3001	-	3,4,4	2.15	3 (100%)	3,6,6	1.35	0
3	PLR	B	1001	1	15,15,15	1.01	1 (6%)	21,22,22	1.40	3 (14%)
4	TS6	A	3001	-	3,4,4	2.12	3 (100%)	3,6,6	1.40	0
5	SEP	D	2001[A]	-	9,10,10	1.70	2 (22%)	9,14,14	2.03	2 (22%)
3	PLR	C	1001	1	15,15,15	0.97	1 (6%)	21,22,22	1.12	2 (9%)
3	PLR	A	1001	1	15,15,15	0.99	1 (6%)	21,22,22	1.04	1 (4%)

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	PLR	D	1001	1	-	1/6/6/6	0/1/1/1
5	SEP	D	2002	-	-	7/10/10/10	-
5	SEP	D	2001[B]	-	-	4/10/10/10	-
5	SEP	B	2001[A]	-	-	5/10/10/10	-
5	SEP	B	2001[B]	-	-	3/10/10/10	-
5	SEP	B	2002	-	-	7/10/10/10	-
3	PLR	B	1001	1	-	0/6/6/6	0/1/1/1
5	SEP	D	2001[A]	-	-	1/10/10/10	-
3	PLR	C	1001	1	-	3/6/6/6	0/1/1/1
3	PLR	A	1001	1	-	0/6/6/6	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	2002	SEP	P-O1P	3.66	1.61	1.50
5	D	2001[A]	SEP	P-O1P	3.60	1.61	1.50
5	B	2002	SEP	P-O1P	3.60	1.61	1.50
5	B	2001[A]	SEP	P-O1P	3.56	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2001[B]	SEP	P-O1P	3.53	1.61	1.50
5	D	2001[B]	SEP	P-O1P	3.51	1.61	1.50
3	D	1001	PLR	C2-N1	2.44	1.38	1.33
3	B	1001	PLR	C2-N1	2.42	1.38	1.33
3	A	1001	PLR	C2-N1	2.30	1.38	1.33
4	A	3002	TS6	P-O1P	2.26	1.51	1.46
4	C	3001	TS6	P-O1P	2.23	1.51	1.46
5	D	2002	SEP	OXT-C	-2.21	1.23	1.30
5	B	2002	SEP	OXT-C	-2.21	1.23	1.30
3	C	1001	PLR	C2-N1	2.21	1.37	1.33
5	D	2001[A]	SEP	OXT-C	-2.19	1.23	1.30
4	A	3001	TS6	P-O1P	2.18	1.51	1.46
5	D	2001[B]	SEP	OXT-C	-2.17	1.23	1.30
5	B	2001[A]	SEP	OXT-C	-2.16	1.23	1.30
4	C	3001	TS6	P-O4P	-2.14	1.51	1.56
4	A	3002	TS6	P-O4P	-2.12	1.51	1.56
5	B	2001[B]	SEP	OXT-C	-2.11	1.23	1.30
4	A	3001	TS6	P-O4P	-2.10	1.51	1.56
4	A	3001	TS6	P-O3P	-2.08	1.51	1.56
4	C	3001	TS6	P-O3P	-2.07	1.51	1.56
4	A	3002	TS6	P-O3P	-2.02	1.51	1.56

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	2001[A]	SEP	OG-CB-CA	4.88	112.31	108.06
5	B	2002	SEP	OG-CB-CA	4.47	111.96	108.06
5	B	2001[A]	SEP	OG-CB-CA	3.87	111.43	108.06
5	D	2002	SEP	OG-CB-CA	3.50	111.11	108.06
3	B	1001	PLR	C4A-C4-C5	3.43	124.47	120.94
5	D	2001[B]	SEP	OG-CB-CA	3.28	110.91	108.06
5	B	2001[B]	SEP	OG-CB-CA	3.24	110.89	108.06
3	B	1001	PLR	O4P-C5A-C5	2.88	114.76	109.36
3	C	1001	PLR	C6-C5-C4	2.79	120.38	118.10
5	D	2001[A]	SEP	OXT-C-O	-2.78	117.78	124.08
5	D	2002	SEP	OXT-C-O	-2.74	117.85	124.08
5	B	2001[A]	SEP	OXT-C-O	-2.70	117.95	124.08
5	B	2002	SEP	OXT-C-O	-2.69	117.98	124.08
5	D	2001[B]	SEP	OXT-C-O	-2.56	118.28	124.08
3	C	1001	PLR	O4P-C5A-C5	2.49	114.02	109.36
5	B	2001[B]	SEP	OXT-C-O	-2.45	118.53	124.08
3	D	1001	PLR	O4P-C5A-C5	2.36	113.78	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	PLR	C6-C5-C4	2.33	120.01	118.10
3	B	1001	PLR	C4A-C4-C3	-2.29	116.71	120.52

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1001	PLR	C4-C5-C5A-O4P
3	C	1001	PLR	C6-C5-C5A-O4P
5	B	2001[A]	SEP	N-CA-CB-OG
5	B	2001[A]	SEP	CB-OG-P-O2P
5	B	2001[A]	SEP	CB-OG-P-O3P
5	B	2001[B]	SEP	CB-OG-P-O3P
5	B	2002	SEP	N-CA-CB-OG
5	B	2002	SEP	O-C-CA-N
5	B	2002	SEP	CB-OG-P-O1P
5	B	2002	SEP	CB-OG-P-O2P
5	B	2002	SEP	CB-OG-P-O3P
5	D	2001[B]	SEP	CB-OG-P-O1P
5	D	2001[B]	SEP	CB-OG-P-O2P
5	D	2001[B]	SEP	CB-OG-P-O3P
5	D	2002	SEP	N-CA-CB-OG
5	D	2002	SEP	CB-OG-P-O3P
5	B	2002	SEP	OXT-C-CA-N
5	B	2001[A]	SEP	CB-OG-P-O1P
5	D	2002	SEP	CB-OG-P-O1P
5	D	2002	SEP	O-C-CA-N
5	D	2002	SEP	CB-OG-P-O2P
3	D	1001	PLR	C4-C5-C5A-O4P
5	D	2001[A]	SEP	N-CA-CB-OG
5	D	2001[B]	SEP	CA-CB-OG-P
5	B	2001[B]	SEP	CB-OG-P-O1P
5	B	2001[A]	SEP	C-CA-CB-OG
5	D	2002	SEP	OXT-C-CA-N
3	C	1001	PLR	C5A-O4P-P-O3P
5	B	2001[B]	SEP	CB-OG-P-O2P
5	B	2002	SEP	CA-CB-OG-P
5	D	2002	SEP	CA-CB-OG-P

There are no ring outliers.

9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1001	PLR	1	0
5	D	2001[B]	SEP	3	0
5	B	2001[A]	SEP	2	0
5	B	2001[B]	SEP	2	0
5	B	2002	SEP	1	0
3	B	1001	PLR	1	0
5	D	2001[A]	SEP	2	0
3	C	1001	PLR	3	0
3	A	1001	PLR	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	441/501 (88%)	-1.61	0	100	100	30, 52, 86, 117	6 (1%)
1	B	443/501 (88%)	-1.56	0	100	100	30, 54, 87, 136	5 (1%)
1	C	445/501 (88%)	-1.60	0	100	100	33, 52, 88, 113	3 (0%)
1	D	441/501 (88%)	-1.56	0	100	100	28, 53, 87, 141	6 (1%)
2	E	82/90 (91%)	-0.52	2 (2%)	59	49	33, 47, 52, 56	82 (100%)
All	All	1852/2094 (88%)	-1.54	2 (0%)	92	90	28, 52, 87, 141	102 (5%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	75[A]	C	2.2
2	E	74[A]	C	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 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(\AA^2)	Q<0.9
4	TS6	C	3001	5/5	0.97	0.15	65,71,79,84	5
5	SEP	B	2002	11/11	0.97	0.05	66,75,86,90	11
4	TS6	A	3001	5/5	0.98	0.10	61,66,83,86	5
5	SEP	B	2001[A]	11/11	0.98	0.06	65,75,83,88	11
5	SEP	B	2001[B]	11/11	0.98	0.06	65,68,78,78	11
4	TS6	A	3002	5/5	0.98	0.11	57,65,74,80	5
5	SEP	D	2001[A]	11/11	0.98	0.07	71,79,86,95	11
5	SEP	D	2001[B]	11/11	0.98	0.07	63,67,77,78	11
5	SEP	D	2002	11/11	0.98	0.04	63,72,85,85	11
3	PLR	D	1001	15/15	0.99	0.04	46,52,57,61	0
3	PLR	B	1001	15/15	1.00	0.03	46,52,57,57	0
3	PLR	C	1001	15/15	1.00	0.02	45,53,60,61	0
3	PLR	A	1001	15/15	1.00	0.03	44,49,55,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.