Full wwPDB X-ray Structure Validation Report (i)

Jun 11, 2024 – 06:32 PM EDT

PDB ID	:	2CT8
Title	:	Crystal structure of Aquifex aeolicus methionyl-tRNA synthetase complexed with tRNA(Met) and methionyl-adenylate anologue
Authors	:	Nakanishi, K.; Ogiso, Y.; Nakama, T.; Fukai, S.; Nureki, O.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2005-05-23
Resolution	:	2.70 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 (i) 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 (i)) were used in the production of this report:

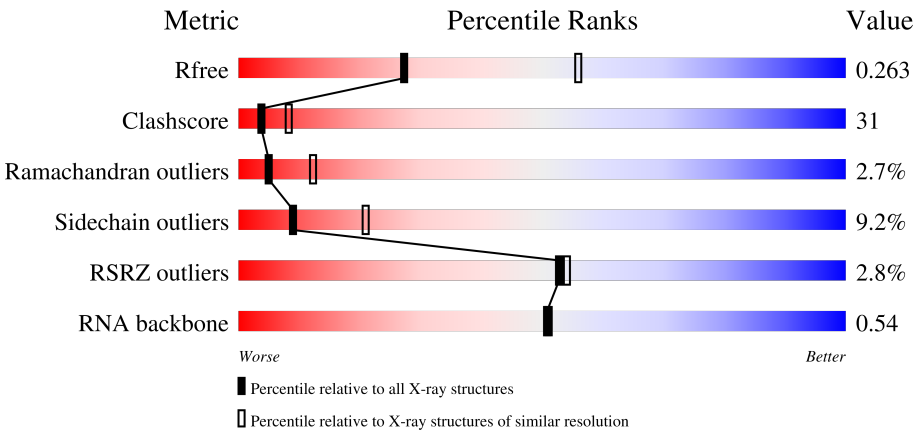
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)
RNA backbone	3102	1159 (3.00-2.40)

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 <=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	C	74	12% 11% 61% 27% •
1	D	74	11% 30% 32% 35% •
2	A	497	% 47% 39% 7% • 6%

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Mol	Chain	Length	Quality of chain
2	B	497	% 45% 40% 7% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MSP	A	501	X	-	-	-
3	MSP	B	1501	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11134 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.

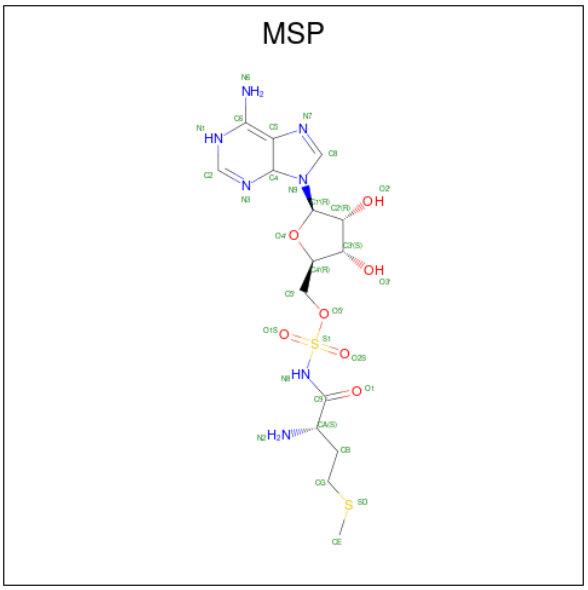
- Molecule 1 is a RNA chain called RNA (74-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	C	74	1583	704	285	520	74	0	0	0
1	D	74	1583	704	285	520	74	0	0	0

- Molecule 2 is a protein called Methionyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	465	3914	2566	638	701	9	0	0	0
2	B	465	3914	2566	638	701	9	0	0	0

- Molecule 3 is 5'-O-[(L-METHIONYL)-SULPHAMOYL]ADENOSINE (three-letter code: MSP) (formula: $C_{15}H_{25}N_7O_7S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	31	15	7	7	2	0	0
3	B	1	31	15	7	7	2	0	0

- Molecule 4 is water.

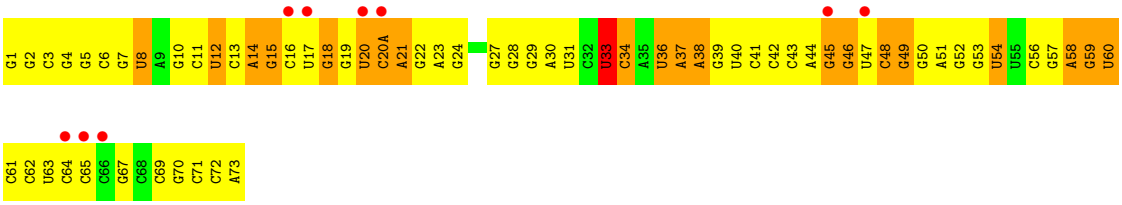
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	C	5	5	5	0	0
4	D	14	14	14	0	0
4	A	29	29	29	0	0
4	B	30	30	30	0	0

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.

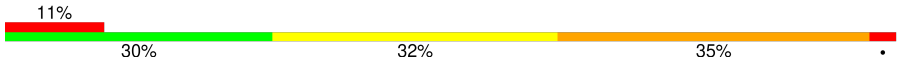
- Molecule 1: RNA (74-MER)

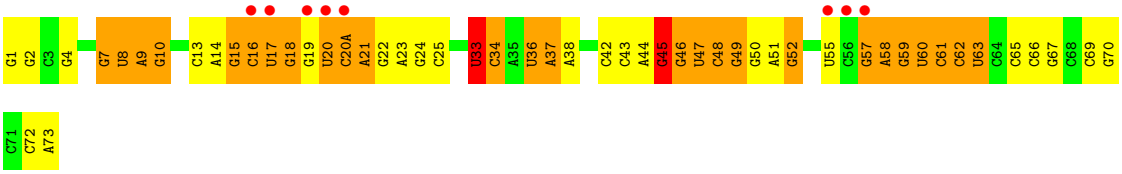
Chain C:



- Molecule 1: RNA (74-MER)

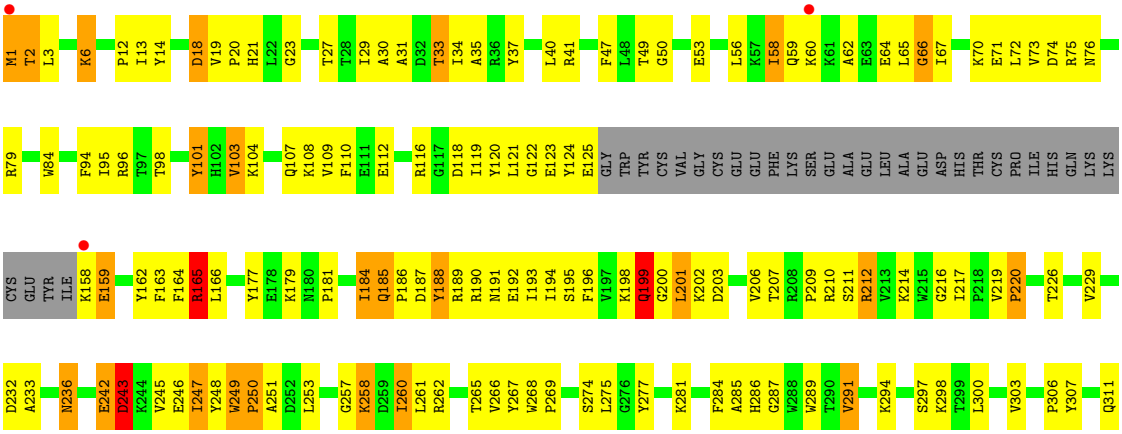
Chain D:





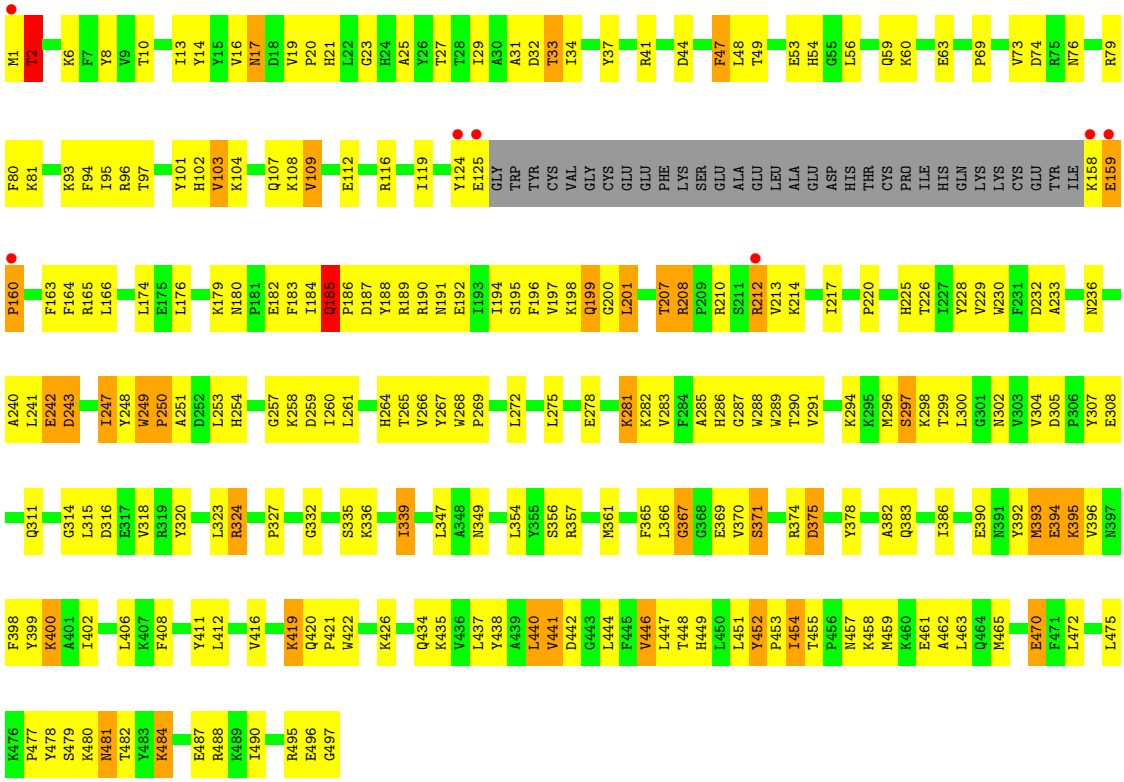
- Molecule 2: Methionyl-tRNA synthetase

Chain A:



- Molecule 2: Methionyl-tRNA synthetase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	91.49Å 110.61Å 161.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.83 – 2.70 48.29 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.2 (37.83-2.70) 93.3 (48.29-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.98 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.272 0.211 , 0.263	Depositor DCC
R_{free} test set	3006 reflections (7.07%)	wwPDB-VP
Wilson B-factor (Å^2)	41.5	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 44.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11134	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MSP

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	C	0.35	1/1768 (0.1%)	0.72	1/2754 (0.0%)
1	D	0.39	1/1768 (0.1%)	0.75	2/2754 (0.1%)
2	A	0.43	0/4021	0.65	1/5426 (0.0%)
2	B	0.47	0/4021	0.69	3/5426 (0.1%)
All	All	0.43	2/11578 (0.0%)	0.69	7/16360 (0.0%)

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	D	0	1
2	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1	G	OP3-P	-7.29	1.52	1.61
1	D	1	G	OP3-P	-7.21	1.52	1.61

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	185	GLN	C-N-CD	6.40	141.84	128.40
1	D	45	G	C2'-C3'-O3'	5.96	123.23	113.70
2	B	185	GLN	N-CA-C	5.74	126.48	111.00
1	D	33	U	N1-C1'-C2'	5.71	121.43	114.00
1	C	33	U	N1-C1'-C2'	5.38	120.99	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	185	GLN	C-N-CA	-5.30	99.73	122.00
2	A	184	ILE	N-CA-C	-5.04	97.38	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	452	TYR	Sidechain
1	D	33	U	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	C	1583	0	802	86	0
1	D	1583	0	802	78	0
2	A	3914	0	3913	240	0
2	B	3914	0	3913	242	0
3	A	31	0	24	6	0
3	B	31	0	24	6	0
4	A	29	0	0	2	0
4	B	30	0	0	2	0
4	C	5	0	0	0	0
4	D	14	0	0	1	0
All	All	11134	0	9478	633	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 31.

All (633) 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:51:A:H2'	1:D:52:G:H5"	1.24	1.12
1:C:59:G:H2'	1:C:60:U:H5'	1.43	1.00
2:B:448:THR:HA	2:B:459:MET:CE	1.93	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:A:H61	1:C:46:G:H2'	1.28	0.97
2:A:485:LEU:H	2:A:485:LEU:HD23	1.27	0.97
2:B:448:THR:HA	2:B:459:MET:HE3	1.45	0.97
1:D:61:C:H2'	1:D:62:C:H5"	1.48	0.96
2:B:208:ARG:NH1	2:B:212:ARG:HD3	1.82	0.93
2:A:189:ARG:NH2	2:A:258:LYS:HD2	1.83	0.93
2:A:370:VAL:HG21	2:A:441:VAL:HG11	1.50	0.93
1:C:11:C:H2'	1:C:12:U:H5"	1.48	0.92
1:D:51:A:C2'	1:D:52:G:H5"	2.01	0.91
2:A:107:GLN:HB3	2:A:220:PRO:HG3	1.51	0.90
2:B:21:HIS:HD2	2:B:23:GLY:H	1.20	0.90
2:A:355:TYR:HB3	2:A:465:MET:HE1	1.51	0.90
1:D:62:C:H2'	1:D:63:U:H5"	1.55	0.89
2:B:249:TRP:O	2:B:251:ALA:N	2.06	0.89
2:A:386:ILE:HD12	2:A:475:LEU:HB2	1.53	0.88
2:A:449:HIS:HE1	2:A:472:LEU:H	1.22	0.86
2:A:29:ILE:O	2:A:33:THR:HG22	1.76	0.84
2:B:437:LEU:O	2:B:441:VAL:HG13	1.77	0.84
2:B:210:ARG:HH21	2:B:214:LYS:HE2	1.43	0.84
1:C:53:G:H2'	1:C:54:U:H5"	1.58	0.84
2:B:289:TRP:H	3:B:1501:MSP:HN1	1.26	0.84
2:A:191:ASN:HA	2:A:194:ILE:HG12	1.59	0.84
2:A:162:TYR:H	2:A:207:THR:HG22	1.43	0.82
2:B:159:GLU:HG3	2:B:159:GLU:O	1.77	0.82
2:B:208:ARG:HH11	2:B:212:ARG:HD3	1.40	0.82
2:B:2:THR:HG21	2:B:247:ILE:HA	1.62	0.82
2:B:361:MET:CE	2:B:421:PRO:HG2	2.09	0.81
2:B:25:ALA:O	2:B:29:ILE:HG12	1.79	0.81
2:B:17:ASN:N	2:B:17:ASN:HD22	1.78	0.81
2:B:29:ILE:O	2:B:33:THR:HG22	1.80	0.81
2:A:75:ARG:HD2	2:B:336:LYS:NZ	1.96	0.81
2:A:428:ARG:O	2:A:428:ARG:HG2	1.80	0.80
2:A:485:LEU:H	2:A:485:LEU:CD2	1.94	0.80
2:B:194:ILE:HG13	2:B:195:SER:N	1.96	0.80
2:A:257:GLY:H	2:A:260:ILE:HD11	1.44	0.80
2:B:249:TRP:O	2:B:250:PRO:C	2.20	0.79
2:B:305:ASP:HB3	2:B:308:GLU:HG2	1.65	0.79
1:C:11:C:C2'	1:C:12:U:H5"	2.12	0.78
2:B:361:MET:HE1	2:B:421:PRO:HG2	1.65	0.78
2:A:289:TRP:H	3:A:501:MSP:HN1	1.30	0.77
2:B:107:GLN:HB3	2:B:220:PRO:HG3	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:TYR:HD2	3:B:1501:MSP:H5'1	1.50	0.77
2:B:20:PRO:HB3	2:B:80:PHE:CE1	2.20	0.77
2:A:188:TYR:O	2:A:192:GLU:HG3	1.85	0.76
2:B:103:VAL:HB	2:B:217:ILE:HD12	1.66	0.76
2:B:242:GLU:O	2:B:243:ASP:HB3	1.86	0.76
1:C:20(A):C:H3'	1:C:21:A:H4'	1.66	0.76
2:A:307:TYR:O	2:A:311:GLN:HG2	1.86	0.76
1:C:42:C:H2'	1:C:43:C:C6	2.20	0.75
2:A:79:ARG:NH1	2:B:497:GLY:HA2	2.01	0.75
2:A:75:ARG:HD2	2:B:336:LYS:HZ3	1.50	0.75
2:A:355:TYR:HB3	2:A:465:MET:CE	2.15	0.75
1:D:61:C:C2'	1:D:62:C:H5"	2.16	0.75
1:D:62:C:C2'	1:D:63:U:H5"	2.16	0.75
2:A:249:TRP:O	2:A:251:ALA:N	2.19	0.74
1:D:7:G:H5"	1:D:8:U:OP2	1.88	0.74
2:A:200:GLY:O	2:A:201:LEU:HB2	1.83	0.74
2:B:2:THR:CG2	2:B:247:ILE:HA	2.17	0.74
1:D:49:G:H1	1:D:65:C:H42	1.33	0.74
1:D:48:C:O2'	1:D:49:G:OP2	2.04	0.74
2:B:184:ILE:HG13	2:B:265:THR:HG21	1.69	0.74
2:A:438:TYR:OH	2:A:481:ASN:HA	1.86	0.74
2:B:179:LYS:HE2	2:B:180:ASN:HD21	1.53	0.74
1:D:20:U:H1'	1:D:20(A):C:H3'	1.70	0.74
1:D:44:A:C2'	1:D:45:G:H5'	2.18	0.73
2:B:17:ASN:HD22	2:B:17:ASN:H	1.36	0.73
2:A:249:TRP:O	2:A:250:PRO:C	2.25	0.73
2:A:411:TYR:HA	2:A:414:LYS:HD2	1.70	0.73
2:B:320:TYR:HA	2:B:454:ILE:CD1	2.18	0.73
2:B:383:GLN:O	2:B:386:ILE:HG12	1.89	0.73
2:B:196:PHE:O	2:B:199:GLN:HG3	1.89	0.72
1:C:43:C:O2'	1:C:44:A:H5'	1.88	0.72
2:A:369:GLU:HG3	2:A:484:LYS:HD2	1.71	0.72
2:A:320:TYR:HA	2:A:454:ILE:HD11	1.71	0.72
2:A:386:ILE:HD12	2:A:475:LEU:CB	2.19	0.72
2:A:2:THR:CG2	2:A:247:ILE:HA	2.20	0.72
2:A:101:TYR:H	2:A:101:TYR:HD1	1.35	0.71
2:A:449:HIS:CE1	2:A:472:LEU:H	2.09	0.71
2:B:56:LEU:HG	2:B:60:LYS:HE3	1.72	0.70
2:B:184:ILE:HB	2:B:190:ARG:CB	2.21	0.70
2:B:261:LEU:HD13	2:B:285:ALA:HB2	1.72	0.70
1:D:47:U:H2'	1:D:50:G:OP1	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:485:LEU:HD23	2:A:485:LEU:N	2.04	0.70
1:C:18:G:H1'	1:C:58:A:C2	2.27	0.70
2:B:21:HIS:HD2	2:B:23:GLY:N	1.90	0.70
1:D:13:C:O2'	1:D:14:A:H5'	1.92	0.69
2:B:184:ILE:HB	2:B:190:ARG:HB2	1.74	0.69
2:B:369:GLU:HG2	2:B:484:LYS:HG2	1.74	0.69
2:B:458:LYS:HE2	4:B:1513:HOH:O	1.92	0.69
1:D:9:A:H5"	1:D:10:G:OP2	1.92	0.69
2:B:296:MET:HA	2:B:302:ASN:OD1	1.93	0.69
1:C:42:C:H2'	1:C:43:C:H6	1.56	0.68
2:B:213:VAL:O	2:B:226:THR:HG21	1.93	0.68
1:C:69:C:H2'	1:C:70:G:H8	1.58	0.68
2:A:359:VAL:HG13	2:A:485:LEU:HD12	1.74	0.68
2:A:31:ALA:O	2:A:34:ILE:HG22	1.93	0.68
2:B:438:TYR:OH	2:B:481:ASN:HA	1.94	0.68
2:B:208:ARG:HH11	2:B:212:ARG:CD	2.06	0.68
1:D:19:G:O4'	1:D:57:G:N2	2.26	0.68
1:C:20:U:O3'	1:C:20(A):C:H4'	1.94	0.67
2:B:21:HIS:CD2	2:B:23:GLY:H	2.07	0.67
2:A:58:ILE:HD13	2:A:58:ILE:O	1.95	0.67
2:B:335:SER:O	2:B:339:ILE:HG13	1.94	0.67
1:D:15:G:H2'	1:D:59:G:H1	1.58	0.67
2:A:193:ILE:C	2:A:195:SER:H	1.98	0.67
1:D:58:A:H2'	1:D:60:U:OP2	1.94	0.67
2:A:70:LYS:HD2	2:A:74:ASP:OD2	1.94	0.67
1:C:29:G:O2'	1:C:30:A:H5'	1.94	0.67
2:A:162:TYR:H	2:A:207:THR:CG2	2.07	0.67
1:D:23:A:H2'	1:D:24:G:H8	1.60	0.66
1:D:36:U:H4'	1:D:37:A:OP1	1.94	0.66
2:B:179:LYS:CE	2:B:180:ASN:HD21	2.08	0.66
2:B:250:PRO:HG3	2:B:278:GLU:HG2	1.78	0.66
1:D:62:C:C3'	1:D:63:U:H5"	2.25	0.66
2:A:109:VAL:HG13	2:A:275:LEU:HD11	1.78	0.66
2:A:268:TRP:HB3	2:A:269:PRO:HD3	1.78	0.66
2:B:200:GLY:O	2:B:201:LEU:HB2	1.95	0.66
2:B:257:GLY:HA3	3:B:1501:MSP:O2'	1.96	0.66
1:D:38:A:O3'	2:B:349:ASN:HB3	1.96	0.66
2:B:210:ARG:NH2	2:B:214:LYS:HE2	2.10	0.66
2:B:336:LYS:HA	2:B:339:ILE:HD12	1.78	0.66
2:A:119:ILE:HD13	2:A:164:PHE:HA	1.77	0.65
1:D:58:A:H1'	1:D:60:U:H5	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:107:GLN:CB	2:A:220:PRO:HG3	2.25	0.65
2:A:351:ILE:HD13	2:A:409:THR:HG21	1.79	0.65
2:B:33:THR:HG21	2:B:323:LEU:HD11	1.77	0.65
1:C:14:A:H2'	1:C:15:G:O4'	1.96	0.64
2:A:14:TYR:HD2	3:A:501:MSP:H5'1	1.63	0.64
1:C:7:G:H5"	1:C:8:U:OP2	1.98	0.64
2:A:198:LYS:O	2:A:199:GLN:HB3	1.97	0.64
2:A:242:GLU:O	2:A:243:ASP:HB3	1.97	0.64
2:A:1:MET:O	2:A:2:THR:HG23	1.98	0.64
2:A:184:ILE:HD12	2:A:190:ARG:HG3	1.80	0.64
2:A:185:GLN:O	2:A:187:ASP:N	2.31	0.64
2:A:316:ASP:HB3	2:A:455:THR:OG1	1.97	0.64
1:C:21:A:N6	1:C:46:G:H2'	2.08	0.63
2:A:420:GLN:HB2	2:A:422:TRP:CZ2	2.34	0.63
2:B:324:ARG:HB2	2:B:402:ILE:HD13	1.79	0.63
1:C:18:G:H2'	1:C:57:G:N2	2.14	0.63
1:D:38:A:H4'	2:B:349:ASN:OD1	1.99	0.63
2:B:37:TYR:OH	2:B:390:GLU:HG2	1.98	0.63
2:A:427:GLU:O	2:A:428:ARG:HB3	1.97	0.63
2:B:17:ASN:H	2:B:17:ASN:ND2	1.97	0.62
2:A:2:THR:HG21	2:A:247:ILE:HA	1.80	0.62
2:B:124:TYR:O	2:B:158:LYS:N	2.31	0.62
1:C:36:U:H4'	1:C:37:A:OP1	1.97	0.62
2:A:405:ILE:CD1	2:A:450:LEU:HB3	2.29	0.62
1:C:59:G:H2'	1:C:60:U:C5'	2.23	0.62
2:A:186:PRO:HB2	2:A:189:ARG:HG2	1.82	0.62
1:C:53:G:C2'	1:C:54:U:H5"	2.29	0.62
2:A:335:SER:O	2:A:339:ILE:HG13	2.00	0.62
2:B:19:VAL:HB	2:B:79:ARG:HH21	1.65	0.62
2:A:185:GLN:HA	2:A:185:GLN:OE1	1.98	0.61
2:B:184:ILE:HG21	2:B:190:ARG:HA	1.82	0.61
1:C:69:C:H2'	1:C:70:G:C8	2.35	0.61
1:D:61:C:H6	1:D:61:C:H5'	1.64	0.61
2:B:2:THR:HG21	2:B:247:ILE:CA	2.29	0.61
1:C:2:G:N2	1:C:72:C:H1'	2.16	0.61
1:D:49:G:H1	1:D:65:C:N4	1.98	0.61
2:A:242:GLU:O	2:A:242:GLU:HG2	1.99	0.61
2:B:297:SER:HB3	2:B:300:LEU:HD23	1.81	0.61
2:B:296:MET:HE3	2:B:304:VAL:H	1.66	0.61
2:B:395:LYS:NZ	2:B:395:LYS:HB3	2.16	0.61
2:A:249:TRP:HB3	2:A:250:PRO:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:TYR:CD2	3:B:1501:MSP:H5'1	2.35	0.60
2:A:266:VAL:O	2:A:269:PRO:HD2	2.01	0.60
2:B:166:LEU:HG	2:B:201:LEU:HD13	1.82	0.60
2:A:193:ILE:HD13	2:A:265:THR:OG1	2.01	0.60
2:B:101:TYR:CZ	2:B:242:GLU:HG3	2.36	0.60
2:B:297:SER:HB3	2:B:300:LEU:CD2	2.31	0.60
1:D:20(A):C:H4'	1:D:21:A:O5'	2.01	0.60
2:B:76:ASN:ND2	2:B:79:ARG:NH1	2.49	0.60
2:A:2:THR:HG21	2:A:247:ILE:HB	1.82	0.60
1:D:52:G:O6	1:D:62:C:N4	2.34	0.60
2:B:17:ASN:N	2:B:17:ASN:ND2	2.48	0.60
1:C:23:A:H2'	1:C:24:G:H8	1.65	0.60
2:A:37:TYR:O	2:A:41:ARG:HG2	2.01	0.60
2:A:107:GLN:HB3	2:A:220:PRO:CG	2.28	0.60
2:B:185:GLN:OE1	2:B:185:GLN:HA	2.02	0.60
2:B:449:HIS:HE1	2:B:472:LEU:H	1.47	0.60
1:D:20:U:C1'	1:D:20(A):C:H3'	2.31	0.60
2:A:423:ALA:O	2:A:427:GLU:HG3	2.02	0.60
2:B:124:TYR:CD1	2:B:125:GLU:N	2.69	0.60
1:C:59:G:C2'	1:C:60:U:H5'	2.28	0.59
1:D:23:A:H2'	1:D:24:G:C8	2.37	0.59
1:C:58:A:H1'	1:C:60:U:H5	1.66	0.59
2:A:166:LEU:HG	2:A:201:LEU:HD12	1.83	0.59
2:B:44:ASP:OD2	2:B:247:ILE:HD11	2.02	0.59
2:B:31:ALA:O	2:B:34:ILE:HG22	2.03	0.59
1:C:53:G:H2'	1:C:54:U:C5'	2.29	0.59
2:A:58:ILE:O	2:A:62:ALA:HB2	2.02	0.59
2:A:257:GLY:HA3	3:A:501:MSP:O2'	2.03	0.59
2:A:286:HIS:HA	2:A:329:GLY:HA2	1.85	0.59
1:D:58:A:H1'	1:D:60:U:C5	2.37	0.59
2:A:193:ILE:HD11	2:A:261:LEU:HG	1.85	0.59
2:B:316:ASP:OD2	2:B:457:ASN:HB2	2.03	0.59
2:B:242:GLU:O	2:B:242:GLU:HG2	2.01	0.58
2:B:316:ASP:OD2	2:B:458:LYS:HG2	2.03	0.58
2:A:311:GLN:HB3	2:B:461:GLU:OE2	2.03	0.58
1:C:38:A:H4'	2:A:349:ASN:OD1	2.03	0.58
2:A:210:ARG:NH2	2:A:214:LYS:HD3	2.18	0.58
2:A:364:LYS:HE2	2:A:365:PHE:HE2	1.67	0.58
2:B:268:TRP:HB3	2:B:269:PRO:HD3	1.85	0.58
2:A:121:LEU:HD23	2:A:122:GLY:N	2.17	0.58
2:B:442:ASP:OD1	2:B:477:PRO:O	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:ARG:O	2:B:194:ILE:HG23	2.03	0.58
2:A:118:ASP:OD2	2:A:274:SER:HB2	2.03	0.58
2:A:347:LEU:HD13	2:A:492:PHE:CE2	2.38	0.58
2:B:449:HIS:CE1	2:B:472:LEU:H	2.21	0.58
1:C:13:C:O2'	1:C:14:A:H5"	2.04	0.58
2:A:19:VAL:HG13	2:A:20:PRO:HD2	1.85	0.58
2:A:118:ASP:HA	2:A:165:ARG:HG3	1.86	0.57
2:A:479:SER:O	2:A:480:LYS:HB2	2.04	0.57
2:B:320:TYR:HA	2:B:454:ILE:HD11	1.84	0.57
2:B:37:TYR:CD1	2:B:393:MET:HG2	2.40	0.57
2:B:176:LEU:HD12	2:B:180:ASN:HD22	1.70	0.57
2:A:71:GLU:OE2	2:A:71:GLU:HA	2.04	0.57
2:B:416:VAL:HG22	2:B:440:LEU:HD21	1.86	0.57
2:A:233:ALA:O	2:A:236:ASN:HB3	2.04	0.57
2:B:297:SER:CB	2:B:300:LEU:HD23	2.34	0.57
1:C:30:A:H2'	1:C:31:U:C6	2.40	0.57
1:C:43:C:H2'	1:C:44:A:O4'	2.04	0.57
1:C:58:A:H2'	1:C:60:U:OP2	2.05	0.57
2:B:76:ASN:HA	2:B:79:ARG:HG3	1.86	0.57
2:A:73:VAL:HG12	2:A:96:ARG:HH21	1.69	0.57
2:A:186:PRO:HB2	2:A:189:ARG:CG	2.35	0.57
2:A:294:LYS:HE2	2:A:294:LYS:HA	1.87	0.57
2:B:1:MET:SD	2:B:250:PRO:HB2	2.44	0.57
2:B:354:LEU:O	2:B:357:ARG:HG2	2.05	0.57
2:B:184:ILE:HG13	2:B:265:THR:CG2	2.35	0.57
1:C:62:C:H2'	1:C:63:U:C6	2.39	0.56
1:C:40:U:H2'	1:C:41:C:C6	2.39	0.56
1:C:62:C:H2'	1:C:63:U:H6	1.71	0.56
1:C:3:C:H2'	1:C:4:G:H8	1.70	0.56
1:C:51:A:O2'	1:C:52:G:H5'	2.05	0.56
2:A:189:ARG:CZ	2:A:258:LYS:HD2	2.36	0.56
1:C:36:U:O4	2:A:352:GLY:HA3	2.05	0.56
1:D:20:U:H1'	1:D:20(A):C:C3'	2.34	0.56
2:A:112:GLU:O	2:A:116:ARG:HG3	2.06	0.56
2:B:107:GLN:HB3	2:B:220:PRO:CG	2.36	0.56
2:A:260:ILE:HD13	2:A:260:ILE:H	1.71	0.56
2:A:420:GLN:O	2:A:420:GLN:HG3	2.06	0.56
1:C:18:G:H2'	1:C:57:G:H21	1.70	0.56
1:D:62:C:H3'	1:D:63:U:H5"	1.88	0.56
2:A:2:THR:HG21	2:A:247:ILE:CB	2.35	0.56
2:A:60:LYS:NZ	2:A:60:LYS:HB2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:LYS:O	2:B:108:LYS:HG3	2.06	0.56
1:C:50:G:H2'	1:C:51:A:O4'	2.06	0.56
2:A:177:TYR:CD1	2:A:194:ILE:HG22	2.41	0.56
2:B:184:ILE:N	2:B:184:ILE:HD12	2.20	0.56
2:A:286:HIS:HD2	2:A:287:GLY:O	1.89	0.55
1:D:47:U:O2'	1:D:48:C:OP1	2.21	0.55
2:A:27:THR:OG1	2:A:286:HIS:HE1	1.89	0.55
1:C:44:A:N3	1:C:44:A:H2'	2.20	0.55
2:A:437:LEU:O	2:A:441:VAL:HG12	2.06	0.55
1:C:8:U:H6	1:C:8:U:H5'	1.72	0.55
1:C:23:A:H2'	1:C:24:G:C8	2.41	0.55
1:C:43:C:C2'	1:C:44:A:H5'	2.36	0.55
2:B:189:ARG:NH2	2:B:258:LYS:HE2	2.22	0.55
2:B:356:SER:O	2:B:488:ARG:HD2	2.07	0.55
2:B:19:VAL:CG2	2:B:20:PRO:HD2	2.37	0.55
2:B:103:VAL:HB	2:B:217:ILE:CD1	2.36	0.55
2:B:305:ASP:HB3	2:B:308:GLU:CG	2.35	0.54
1:D:44:A:H2'	1:D:45:G:H5'	1.89	0.54
2:B:179:LYS:HE2	2:B:180:ASN:ND2	2.23	0.54
1:D:58:A:O2'	1:D:59:G:O5'	2.22	0.54
1:D:73:A:N3	1:D:73:A:H2'	2.22	0.54
2:A:455:THR:O	2:A:455:THR:HG23	2.08	0.54
2:A:179:LYS:O	2:A:181:PRO:HD3	2.07	0.54
2:B:208:ARG:NH1	2:B:212:ARG:CD	2.63	0.54
2:A:21:HIS:HD2	2:A:23:GLY:N	2.06	0.54
1:C:60:U:H5"	1:C:61:C:OP2	2.08	0.54
2:A:76:ASN:HA	2:A:79:ARG:CG	2.38	0.54
2:B:448:THR:HA	2:B:459:MET:HE2	1.87	0.54
1:C:12:U:H6	1:C:12:U:H5'	1.73	0.54
1:D:20(A):C:O2'	1:D:21:A:OP2	2.25	0.54
1:D:60:U:H2'	1:D:61:C:OP1	2.08	0.54
2:A:336:LYS:HE2	2:A:497:GLY:O	2.09	0.53
2:B:289:TRP:N	3:B:1501:MSP:HN1	2.03	0.53
2:B:382:ALA:O	2:B:386:ILE:HG23	2.08	0.53
2:B:324:ARG:C	2:B:324:ARG:HD3	2.29	0.53
2:B:290:THR:HB	2:B:294:LYS:O	2.09	0.53
2:B:327:PRO:HA	2:B:399:TYR:HB2	1.90	0.53
2:B:371:SER:O	2:B:434:GLN:HB3	2.07	0.53
2:A:442:ASP:OD1	2:A:477:PRO:O	2.25	0.53
2:B:393:MET:HE3	2:B:393:MET:HA	1.91	0.53
2:B:470:GLU:OE1	2:B:470:GLU:N	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:64:GLU:C	2:A:66:GLY:H	2.12	0.53
2:B:59:GLN:O	2:B:63:GLU:HG3	2.07	0.53
2:B:336:LYS:HA	2:B:339:ILE:CD1	2.38	0.53
2:B:299:THR:HG23	2:B:300:LEU:HD22	1.91	0.53
2:A:242:GLU:O	2:A:243:ASP:CB	2.57	0.53
2:A:382:ALA:O	2:A:386:ILE:HG22	2.08	0.53
2:B:194:ILE:HG13	2:B:195:SER:H	1.73	0.53
2:A:1:MET:HE1	2:A:281:LYS:HE2	1.91	0.53
2:A:386:ILE:CD1	2:A:475:LEU:HB2	2.32	0.53
2:B:14:TYR:HD2	3:B:1501:MSP:C5'	2.21	0.53
2:A:14:TYR:CD2	3:A:501:MSP:H5'1	2.43	0.52
1:D:63:U:H5'	1:D:63:U:H6	1.73	0.52
2:B:6:LYS:HE2	2:B:248:TYR:O	2.09	0.52
2:B:189:ARG:HA	2:B:192:GLU:OE2	2.09	0.52
2:A:158:LYS:O	2:A:159:GLU:HB2	2.08	0.52
2:A:361:MET:HE3	2:A:422:TRP:HE3	1.75	0.52
2:B:191:ASN:O	2:B:194:ILE:HG12	2.10	0.52
2:B:408:PHE:O	2:B:411:TYR:HB3	2.09	0.52
2:B:208:ARG:HH11	2:B:212:ARG:CG	2.22	0.52
1:C:13:C:H2'	1:C:14:A:H5'	1.91	0.52
2:A:75:ARG:HD2	2:B:336:LYS:HZ2	1.75	0.52
2:A:121:LEU:HB2	2:A:162:TYR:CE1	2.44	0.52
2:A:193:ILE:C	2:A:195:SER:N	2.62	0.52
2:B:2:THR:HG21	2:B:247:ILE:CB	2.40	0.52
2:A:401:ALA:O	2:A:405:ILE:HG12	2.10	0.52
2:A:445:PHE:O	2:A:449:HIS:HD2	1.93	0.52
2:B:101:TYR:CE1	2:B:242:GLU:HG3	2.45	0.52
2:A:2:THR:HG21	2:A:247:ILE:CA	2.40	0.52
1:D:60:U:C2'	1:D:61:C:OP1	2.57	0.51
2:A:49:THR:O	2:A:94:PHE:HA	2.10	0.51
2:A:419:LYS:O	2:A:420:GLN:C	2.49	0.51
2:B:32:ASP:HA	2:B:47:PHE:CE2	2.45	0.51
2:B:191:ASN:HA	2:B:194:ILE:HG12	1.91	0.51
2:A:191:ASN:HA	2:A:194:ILE:CG1	2.35	0.51
2:B:286:HIS:HD2	2:B:287:GLY:O	1.94	0.51
1:C:47:U:H3'	1:C:48:C:H5'	1.92	0.51
1:C:47:U:H3'	1:C:48:C:C5'	2.41	0.51
2:A:196:PHE:CE2	2:A:262:ARG:HD2	2.46	0.51
2:A:1:MET:N	2:A:6:LYS:HE3	2.26	0.51
2:A:266:VAL:C	2:A:269:PRO:HD2	2.30	0.51
1:D:20:U:O2'	1:D:20(A):C:P	2.68	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:G:H2'	1:D:60:U:O4'	2.11	0.51
2:A:198:LYS:O	2:A:199:GLN:CB	2.58	0.51
2:B:249:TRP:C	2:B:249:TRP:CD2	2.84	0.51
1:D:15:G:H4'	1:D:16:C:OP2	2.11	0.51
2:B:393:MET:HA	2:B:393:MET:CE	2.41	0.51
1:D:48:C:HO2'	1:D:49:G:P	2.32	0.51
2:A:336:LYS:HG2	2:A:340:LEU:HD12	1.93	0.50
2:B:95:ILE:HD12	2:B:240:ALA:HB2	1.92	0.50
1:C:2:G:H2'	1:C:3:C:C6	2.46	0.50
2:A:37:TYR:CE1	2:A:41:ARG:NH2	2.80	0.50
2:A:324:ARG:HB2	2:A:402:ILE:HD13	1.93	0.50
1:C:4:G:O2'	1:C:5:G:H5'	2.12	0.50
1:C:19:G:N2	1:C:56:C:C2	2.79	0.50
2:A:186:PRO:HG3	2:A:284:PHE:CE2	2.46	0.50
1:C:11:C:C3'	1:C:12:U:H5"	2.42	0.50
1:D:58:A:O2'	1:D:59:G:P	2.70	0.50
1:C:59:G:N3	1:C:59:G:H5'	2.26	0.50
2:A:327:PRO:HA	2:A:399:TYR:HB2	1.94	0.50
2:A:249:TRP:C	2:A:249:TRP:CD2	2.81	0.50
2:A:196:PHE:O	2:A:199:GLN:HG3	2.11	0.49
2:B:370:VAL:O	2:B:371:SER:HB3	2.12	0.49
2:A:76:ASN:HA	2:A:79:ARG:HG3	1.94	0.49
2:B:19:VAL:HG22	2:B:20:PRO:HD2	1.94	0.49
2:B:37:TYR:CE1	2:B:41:ARG:NH2	2.80	0.49
1:D:20(A):C:O2'	1:D:21:A:C4'	2.60	0.49
2:B:47:PHE:HD1	2:B:48:LEU:N	2.10	0.49
1:C:58:A:O2'	1:C:59:G:P	2.70	0.49
2:A:120:TYR:HD1	2:A:165:ARG:HE	1.59	0.49
2:A:336:LYS:HG2	2:A:340:LEU:CD1	2.43	0.49
2:A:479:SER:O	2:A:480:LYS:CB	2.59	0.49
2:B:104:LYS:HG3	2:B:108:LYS:HE3	1.94	0.49
2:A:185:GLN:O	2:A:186:PRO:C	2.47	0.49
2:B:393:MET:HE1	2:B:398:PHE:HD2	1.78	0.49
2:B:185:GLN:O	2:B:186:PRO:C	2.42	0.49
2:A:40:LEU:HD23	2:A:40:LEU:C	2.32	0.49
2:A:206:VAL:HG22	2:A:206:VAL:O	2.12	0.49
2:B:27:THR:OG1	2:B:286:HIS:HE1	1.94	0.49
2:B:159:GLU:O	2:B:159:GLU:CG	2.54	0.49
2:B:393:MET:HE1	2:B:398:PHE:HA	1.94	0.49
2:A:40:LEU:HD23	2:A:40:LEU:O	2.13	0.48
2:A:12:PRO:HD3	2:A:27:THR:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:389:TYR:CE1	2:A:405:ILE:HD11	2.48	0.48
1:C:36:U:C5	2:A:490:ILE:HG23	2.47	0.48
1:D:33:U:O2'	1:D:34:C:P	2.71	0.48
1:D:61:C:C3'	1:D:62:C:H5"	2.43	0.48
2:A:30:ALA:O	2:A:33:THR:HG23	2.13	0.48
2:A:165:ARG:HA	2:A:203:ASP:OD1	2.13	0.48
2:B:188:TYR:HA	2:B:191:ASN:HD22	1.78	0.48
2:B:307:TYR:O	2:B:311:GLN:HG3	2.13	0.48
1:C:19:G:H1'	1:C:57:G:N3	2.28	0.48
1:D:42:C:O2'	1:D:43:C:H5'	2.12	0.48
2:B:47:PHE:CD1	2:B:47:PHE:C	2.86	0.48
1:D:20:U:O2'	1:D:20(A):C:OP2	2.27	0.48
2:A:21:HIS:HD2	2:A:23:GLY:H	1.60	0.48
1:D:2:G:H1'	4:D:79:HOH:O	2.13	0.48
2:A:261:LEU:HD13	2:A:285:ALA:HB2	1.95	0.48
2:A:297:SER:OG	2:A:300:LEU:HD13	2.13	0.48
2:B:16:VAL:HG21	2:B:73:VAL:HG22	1.94	0.48
2:B:95:ILE:HD13	2:B:236:ASN:HB2	1.96	0.48
1:D:15:G:O2'	1:D:16:C:OP2	2.29	0.48
2:A:357:ARG:O	2:A:361:MET:HG3	2.14	0.48
2:B:183:PHE:HD2	2:B:184:ILE:CD1	2.27	0.48
2:B:496:GLU:O	2:B:497:GLY:O	2.32	0.48
2:A:50:GLY:HA3	2:A:95:ILE:O	2.14	0.48
2:B:16:VAL:HG21	2:B:53:GLU:HG2	1.96	0.48
2:B:374:ARG:NH1	2:B:478:TYR:HB2	2.28	0.48
2:B:452:TYR:HB3	2:B:453:PRO:HD3	1.95	0.48
1:D:24:G:C5	1:D:25:C:C5	3.02	0.47
2:A:359:VAL:HG22	2:A:485:LEU:HD12	1.96	0.47
2:B:314:GLY:O	2:B:318:VAL:HG13	2.15	0.47
2:B:2:THR:HG21	2:B:247:ILE:HB	1.95	0.47
2:A:449:HIS:HE1	2:A:472:LEU:N	2.02	0.47
2:B:13:ILE:HD11	2:B:233:ALA:HB1	1.96	0.47
1:D:19:G:H4'	1:D:20:U:C5	2.50	0.47
2:A:257:GLY:O	2:A:260:ILE:HD13	2.14	0.47
1:C:58:A:O2'	1:C:59:G:O5'	2.33	0.47
1:D:69:C:H2'	1:D:70:G:H8	1.79	0.47
1:D:20(A):C:O2'	1:D:21:A:H4'	2.14	0.47
1:D:19:G:H4'	1:D:20:U:C6	2.50	0.47
1:D:36:U:C4	2:B:490:ILE:HG23	2.50	0.47
2:A:202:LYS:O	2:A:203:ASP:C	2.51	0.47
2:B:112:GLU:O	2:B:116:ARG:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:185:GLN:O	2:B:187:ASP:N	2.46	0.47
2:B:268:TRP:CH2	2:B:272:LEU:HD21	2.50	0.47
2:B:375:ASP:HB2	2:B:435:LYS:HE2	1.97	0.47
1:C:47:U:N3	1:C:50:G:OP1	2.48	0.47
1:D:58:A:O2'	1:D:60:U:H5	1.96	0.47
2:A:247:ILE:HD11	2:A:248:TYR:CZ	2.49	0.47
2:A:291:VAL:O	2:A:334:PHE:O	2.33	0.47
2:A:394:GLU:HB3	4:A:506:HOH:O	2.15	0.47
1:C:19:G:N1	1:C:56:C:N3	2.63	0.47
1:D:44:A:O2'	1:D:45:G:H5'	2.14	0.47
2:A:60:LYS:HB2	2:A:60:LYS:HZ2	1.80	0.47
2:B:207:THR:HG23	2:B:208:ARG:N	2.29	0.47
2:A:14:TYR:HD2	3:A:501:MSP:C5'	2.28	0.47
2:A:405:ILE:HD12	2:A:450:LEU:HB3	1.97	0.47
2:B:19:VAL:HG23	2:B:79:ARG:HE	1.80	0.46
2:B:54:HIS:HD2	2:B:232:ASP:OD2	1.98	0.46
2:B:242:GLU:O	2:B:243:ASP:CB	2.56	0.46
2:B:266:VAL:O	2:B:269:PRO:HD2	2.15	0.46
2:A:487:GLU:HG2	4:A:525:HOH:O	2.16	0.46
2:B:184:ILE:HB	2:B:190:ARG:HB3	1.97	0.46
2:A:1:MET:CE	2:A:281:LYS:HE2	2.45	0.46
2:B:260:ILE:HD12	2:B:264:HIS:HE1	1.80	0.46
1:C:20(A):C:C3'	1:C:21:A:H4'	2.41	0.46
2:A:101:TYR:CD1	2:A:101:TYR:N	2.69	0.46
2:B:103:VAL:CB	2:B:217:ILE:HD12	2.42	0.46
2:B:194:ILE:CG1	2:B:195:SER:N	2.71	0.46
1:C:3:C:H2'	1:C:4:G:C8	2.49	0.46
2:B:109:VAL:HG22	2:B:275:LEU:CD2	2.45	0.46
2:B:164:PHE:O	2:B:166:LEU:N	2.46	0.46
2:B:465:MET:HG3	2:B:487:GLU:O	2.16	0.46
1:C:33:U:O2'	1:C:34:C:OP2	2.31	0.46
1:C:49:G:N3	1:C:49:G:H2'	2.30	0.46
1:D:20:U:H1'	1:D:20(A):C:O3'	2.15	0.46
1:D:48:C:O2'	1:D:49:G:P	2.73	0.46
2:A:21:HIS:HA	2:A:306:PRO:HD3	1.98	0.46
2:A:76:ASN:HA	2:A:79:ARG:HG2	1.98	0.46
2:A:104:LYS:O	2:A:108:LYS:HG3	2.15	0.46
2:A:186:PRO:O	2:A:189:ARG:N	2.48	0.46
2:A:275:LEU:HD13	2:A:277:TYR:CE1	2.51	0.46
2:B:109:VAL:HG22	2:B:275:LEU:CD1	2.46	0.46
2:B:254:HIS:HB2	2:B:283:VAL:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:G:O2'	1:D:46:G:OP1	2.29	0.46
2:B:458:LYS:O	2:B:461:GLU:HB2	2.16	0.46
2:B:472:LEU:HD11	2:B:479:SER:OG	2.15	0.46
1:C:63:U:H2'	1:C:64:C:C6	2.51	0.45
1:C:52:G:H2'	1:C:53:G:O4'	2.16	0.45
2:A:216:GLY:HA3	2:A:226:THR:HG21	1.98	0.45
2:A:210:ARG:O	2:A:210:ARG:HG2	2.16	0.45
1:C:36:U:C4	2:A:490:ILE:HG23	2.52	0.45
1:C:45:G:O2'	1:C:46:G:N7	2.38	0.45
2:B:320:TYR:HA	2:B:454:ILE:HD13	1.98	0.45
2:A:336:LYS:HA	2:A:339:ILE:HD12	1.99	0.45
2:B:390:GLU:O	2:B:394:GLU:HB2	2.16	0.45
1:C:72:C:O2'	1:C:73:A:H5'	2.16	0.45
2:A:289:TRP:N	3:A:501:MSP:HN1	2.06	0.45
2:A:2:THR:HB	2:A:3:LEU:H	1.63	0.45
2:B:228:TYR:CE2	2:B:230:TRP:HB2	2.52	0.45
2:A:294:LYS:HE2	2:A:294:LYS:CA	2.47	0.45
2:A:448:THR:HA	2:A:459:MET:SD	2.57	0.45
2:B:320:TYR:CD1	2:B:347:LEU:HD21	2.51	0.45
1:C:27:G:N2	1:C:44:A:H1'	2.31	0.45
2:A:415:TYR:O	2:A:416:VAL:C	2.55	0.45
2:B:176:LEU:CD1	2:B:180:ASN:HD22	2.30	0.45
1:C:39:G:OP1	2:A:349:ASN:HB3	2.18	0.44
2:B:248:TYR:O	2:B:249:TRP:C	2.55	0.44
1:D:51:A:C3'	1:D:52:G:H5"	2.46	0.44
2:A:382:ALA:O	2:A:386:ILE:CG2	2.66	0.44
2:B:166:LEU:CG	2:B:201:LEU:HD13	2.47	0.44
2:B:448:THR:CA	2:B:459:MET:HE3	2.32	0.44
1:C:7:G:C2	1:C:67:G:C2	3.06	0.44
1:D:43:C:O2'	1:D:44:A:H5'	2.17	0.44
2:A:121:LEU:HD23	2:A:121:LEU:C	2.38	0.44
2:A:53:GLU:HB2	2:A:98:THR:HG23	2.00	0.44
2:A:189:ARG:HH21	2:A:258:LYS:HD2	1.76	0.44
2:A:219:VAL:HA	2:A:220:PRO:HD3	1.84	0.44
2:B:449:HIS:HE1	2:B:472:LEU:N	2.12	0.44
2:B:479:SER:O	2:B:480:LYS:HB2	2.16	0.44
2:A:65:LEU:O	2:A:67:ILE:HG23	2.17	0.44
2:A:249:TRP:CG	2:A:250:PRO:N	2.84	0.44
2:B:119:ILE:HA	2:B:163:PHE:O	2.18	0.44
2:B:212:ARG:H	2:B:212:ARG:HG2	1.27	0.44
2:A:66:GLY:O	2:A:67:ILE:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:110:PHE:CE2	2:A:219:VAL:HG13	2.53	0.44
2:A:185:GLN:OE1	2:A:185:GLN:CA	2.66	0.44
1:D:36:U:H5"	1:D:37:A:OP2	2.18	0.44
2:A:103:VAL:HA	2:A:217:ILE:HD13	2.00	0.44
1:C:15:G:O6	1:C:48:C:O2	2.36	0.43
1:D:18:G:O2'	1:D:19:G:H5'	2.18	0.43
2:A:189:ARG:HA	2:A:189:ARG:HD3	1.76	0.43
2:A:246:GLU:OE1	2:A:246:GLU:HA	2.18	0.43
1:C:28:G:N2	1:C:43:C:C2	2.86	0.43
2:A:65:LEU:O	2:A:66:GLY:C	2.56	0.43
2:A:359:VAL:HG21	2:A:465:MET:HG2	1.99	0.43
2:A:445:PHE:CE1	2:A:468:GLU:HG3	2.53	0.43
2:B:366:LEU:O	2:B:367:GLY:C	2.55	0.43
2:B:395:LYS:HB3	2:B:395:LYS:HZ3	1.81	0.43
1:C:45:G:H5'	1:C:46:G:OP1	2.18	0.43
1:C:71:C:O2'	1:C:72:C:H5'	2.18	0.43
2:A:364:LYS:CE	2:A:365:PHE:HE2	2.31	0.43
2:B:365:PHE:CE1	2:B:422:TRP:HA	2.53	0.43
2:A:193:ILE:CD1	2:A:261:LEU:HG	2.46	0.43
2:A:487:GLU:OE2	2:A:487:GLU:N	2.52	0.43
2:A:95:ILE:HG12	2:A:96:ARG:N	2.34	0.43
2:A:248:TYR:O	2:A:249:TRP:C	2.57	0.43
2:A:314:GLY:O	2:A:318:VAL:HG13	2.19	0.43
2:B:267:TYR:N	2:B:267:TYR:CD2	2.84	0.43
1:C:40:U:H2'	1:C:41:C:H6	1.81	0.43
2:A:314:GLY:O	2:A:318:VAL:CG1	2.66	0.43
1:C:19:G:H5'	1:C:20:U:OP1	2.18	0.43
1:C:20(A):C:H41	1:C:22:G:C1'	2.31	0.43
1:D:9:A:H61	1:D:22:G:H3'	1.82	0.43
2:A:12:PRO:CD	2:A:27:THR:HG21	2.49	0.43
2:A:58:ILE:HD11	2:A:73:VAL:HG23	2.01	0.43
2:A:119:ILE:HA	2:A:163:PHE:O	2.18	0.43
2:A:395:LYS:C	2:A:396:VAL:HG23	2.39	0.43
2:B:93:LYS:CG	2:B:94:PHE:N	2.82	0.43
2:B:197:VAL:C	2:B:199:GLN:H	2.21	0.43
2:A:297:SER:O	2:A:303:VAL:HG23	2.18	0.43
2:B:27:THR:OG1	2:B:286:HIS:CE1	2.72	0.43
2:B:107:GLN:CB	2:B:220:PRO:HG3	2.43	0.43
2:B:197:VAL:O	2:B:199:GLN:N	2.47	0.43
2:A:124:TYR:CG	2:A:125:GLU:N	2.87	0.43
2:B:19:VAL:HB	2:B:79:ARG:NH2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:TYR:O	2:B:41:ARG:HG2	2.18	0.43
2:B:41:ARG:HG2	2:B:41:ARG:HH11	1.83	0.43
2:B:69:PRO:O	2:B:73:VAL:HB	2.18	0.43
1:C:12:U:H2'	1:C:13:C:O4'	2.19	0.42
1:C:41:C:H2'	1:C:42:C:C6	2.54	0.42
2:A:18:ASP:OD2	2:A:298:LYS:HE3	2.19	0.42
2:A:191:ASN:CA	2:A:194:ILE:HG12	2.41	0.42
2:A:326:VAL:HG13	2:A:327:PRO:HD2	2.01	0.42
2:B:182:GLU:O	2:B:282:LYS:HG3	2.19	0.42
2:B:336:LYS:NZ	2:B:497:GLY:OXT	2.46	0.42
2:A:34:ILE:HD12	2:A:34:ILE:HA	1.87	0.42
2:B:386:ILE:HD12	2:B:475:LEU:O	2.19	0.42
2:B:420:GLN:HB2	2:B:422:TRP:CE2	2.54	0.42
1:D:20(A):C:O2'	1:D:21:A:O4'	2.38	0.42
2:A:162:TYR:HD2	2:A:207:THR:HG21	1.84	0.42
2:B:258:LYS:HG3	2:B:259:ASP:N	2.33	0.42
2:A:56:LEU:HD12	2:A:59:GLN:HE21	1.84	0.42
2:A:84:TRP:HA	2:A:84:TRP:CE3	2.55	0.42
2:B:1:MET:O	2:B:2:THR:HG23	2.20	0.42
2:B:490:ILE:HD12	2:B:490:ILE:N	2.34	0.42
2:B:281:LYS:O	2:B:282:LYS:HB2	2.19	0.42
2:B:375:ASP:CB	2:B:435:LYS:HE2	2.49	0.42
2:A:1:MET:H1	2:A:6:LYS:HE3	1.84	0.42
2:A:84:TRP:HA	2:A:84:TRP:HE3	1.85	0.42
2:A:268:TRP:HA	2:A:268:TRP:CE3	2.55	0.42
1:C:54:U:H6	1:C:54:U:H5'	1.84	0.42
1:D:4:G:N2	1:D:70:G:C4	2.88	0.42
2:A:414:LYS:O	2:A:415:TYR:C	2.58	0.42
2:B:48:LEU:HG	2:B:49:THR:N	2.35	0.42
2:B:392:TYR:CG	2:B:400:LYS:HB3	2.55	0.42
1:D:58:A:O2'	1:D:60:U:C5	2.73	0.42
1:D:72:C:O2'	1:D:73:A:H5'	2.20	0.42
2:B:33:THR:HG21	2:B:323:LEU:CD1	2.48	0.42
2:A:19:VAL:HG12	2:A:20:PRO:O	2.20	0.42
2:A:40:LEU:HD22	2:A:41:ARG:HD3	2.01	0.42
2:A:266:VAL:HG12	2:A:267:TYR:HD2	1.85	0.42
2:A:267:TYR:N	2:A:267:TYR:CD2	2.87	0.42
2:B:8:TYR:CE2	2:B:10:THR:HG22	2.55	0.42
2:B:74:ASP:HA	2:B:96:ARG:NH2	2.35	0.42
2:A:34:ILE:CG2	2:A:35:ALA:N	2.83	0.41
2:B:160:PRO:O	2:B:225:HIS:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:C:H2'	1:D:70:G:C8	2.54	0.41
2:B:419:LYS:O	2:B:420:GLN:C	2.59	0.41
1:C:5:G:H2'	1:C:6:C:O4'	2.19	0.41
2:A:159:GLU:HG3	2:A:212:ARG:NH1	2.35	0.41
2:A:179:LYS:C	2:A:181:PRO:HD3	2.40	0.41
2:B:174:LEU:HD23	2:B:174:LEU:HA	1.88	0.41
2:B:207:THR:CG2	2:B:208:ARG:N	2.82	0.41
2:B:361:MET:HE2	2:B:421:PRO:HG2	1.96	0.41
2:B:454:ILE:HG13	2:B:455:THR:HG23	2.03	0.41
1:D:55:U:N3	1:D:57:G:H5"	2.35	0.41
2:A:13:ILE:HG13	2:A:13:ILE:O	2.21	0.41
2:A:493:PRO:O	2:A:495:ARG:N	2.53	0.41
2:B:354:LEU:HG	2:B:444:LEU:HD21	2.02	0.41
2:B:392:TYR:CD1	2:B:400:LYS:HB3	2.55	0.41
1:C:11:C:H6	1:C:11:C:O5'	2.03	0.41
2:A:354:LEU:HG	2:A:444:LEU:HD21	2.02	0.41
2:A:390:GLU:O	2:A:394:GLU:HB2	2.21	0.41
2:B:97:THR:HG22	2:B:102:HIS:NE2	2.35	0.41
2:B:208:ARG:HH12	2:B:212:ARG:HD3	1.80	0.41
1:D:57:G:HO2'	1:D:58:A:P	2.42	0.41
2:A:162:TYR:N	2:A:207:THR:HG22	2.22	0.41
2:A:71:GLU:O	2:A:72:LEU:C	2.59	0.41
2:A:415:TYR:CD2	2:A:440:LEU:HD13	2.56	0.41
2:B:266:VAL:C	2:B:269:PRO:HD2	2.41	0.41
2:B:446:VAL:HG12	2:B:447:LEU:N	2.36	0.41
2:B:451:LEU:HB2	2:B:459:MET:CE	2.51	0.41
1:C:7:G:N2	1:C:67:G:C4	2.89	0.41
1:C:50:G:N2	1:C:65:C:H1'	2.36	0.41
1:D:66:C:O2'	1:D:67:G:H5'	2.21	0.41
2:B:375:ASP:OD1	2:B:378:TYR:HB3	2.20	0.41
2:B:400:LYS:HD2	2:B:400:LYS:HA	1.78	0.41
2:B:482:THR:HG23	2:B:482:THR:O	2.21	0.41
1:C:61:C:H2'	1:C:62:C:C6	2.56	0.41
2:A:311:GLN:OE1	2:A:311:GLN:HA	2.21	0.41
2:A:346:GLU:O	2:A:351:ILE:HG12	2.21	0.41
2:A:451:LEU:HB3	2:A:455:THR:HG22	2.03	0.41
2:B:74:ASP:HA	2:B:96:ARG:HH22	1.86	0.41
2:B:289:TRP:HA	2:B:332:GLY:O	2.20	0.40
2:B:412:LEU:O	2:B:416:VAL:HG23	2.20	0.40
1:D:16:C:H3'	1:D:17:U:H5'	2.02	0.40
2:A:96:ARG:C	2:A:98:THR:H	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:410:SER:O	2:A:414:LYS:HD2	2.21	0.40
2:A:441:VAL:O	2:A:444:LEU:HB2	2.21	0.40
2:B:305:ASP:OD1	2:B:307:TYR:N	2.52	0.40
1:D:63:U:H6	1:D:63:U:C5'	2.33	0.40
2:A:2:THR:HG23	2:A:247:ILE:HA	1.98	0.40
2:A:209:PRO:C	2:A:211:SER:N	2.74	0.40
2:A:214:LYS:O	2:A:214:LYS:HD2	2.21	0.40
2:A:411:TYR:CA	2:A:414:LYS:HD2	2.47	0.40
2:B:241:LEU:O	2:B:242:GLU:C	2.60	0.40
2:B:243:ASP:O	2:B:243:ASP:CG	2.59	0.40
2:B:327:PRO:HG3	2:B:399:TYR:CD2	2.56	0.40
2:B:53:GLU:HB3	2:B:73:VAL:HG21	2.03	0.40
2:B:324:ARG:HD3	2:B:324:ARG:O	2.22	0.40
2:B:375:ASP:HA	4:B:1530:HOH:O	2.21	0.40
2:B:462:ALA:O	2:B:463:LEU:C	2.60	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
2	A	461/497 (93%)	400 (87%)	47 (10%)	14 (3%)	4 10
2	B	461/497 (93%)	419 (91%)	31 (7%)	11 (2%)	6 15
All	All	922/994 (93%)	819 (89%)	78 (8%)	25 (3%)	5 12

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	199	GLN
2	A	249	TRP
2	B	249	TRP

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Mol	Chain	Res	Type
2	B	250	PRO
2	A	250	PRO
2	B	198	LYS
2	B	242	GLU
2	B	367	GLY
2	A	165	ARG
2	A	243	ASP
2	A	396	VAL
2	B	165	ARG
2	B	291	VAL
2	A	66	GLY
2	A	201	LEU
2	A	220	PRO
2	A	242	GLU
2	B	160	PRO
2	A	159	GLU
2	A	291	VAL
2	A	482	THR
2	B	2	THR
2	B	371	SER
2	A	487	GLU
2	B	396	VAL

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
2	A	419/447 (94%)	383 (91%)	36 (9%)	10 24
2	B	419/447 (94%)	378 (90%)	41 (10%)	8 18
All	All	838/894 (94%)	761 (91%)	77 (9%)	9 21

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	1	MET

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Mol	Chain	Res	Type
2	A	2	THR
2	A	6	LYS
2	A	18	ASP
2	A	33	THR
2	A	47	PHE
2	A	58	ILE
2	A	101	TYR
2	A	103	VAL
2	A	123	GLU
2	A	165	ARG
2	A	185	GLN
2	A	188	TYR
2	A	199	GLN
2	A	212	ARG
2	A	229	VAL
2	A	232	ASP
2	A	236	ASN
2	A	243	ASP
2	A	245	VAL
2	A	247	ILE
2	A	253	LEU
2	A	258	LYS
2	A	260	ILE
2	A	315	LEU
2	A	324	ARG
2	A	386	ILE
2	A	393	MET
2	A	406	LEU
2	A	419	LYS
2	A	437	LEU
2	A	440	LEU
2	A	454	ILE
2	A	474	GLU
2	A	482	THR
2	A	485	LEU
2	B	2	THR
2	B	17	ASN
2	B	33	THR
2	B	47	PHE
2	B	81	LYS
2	B	103	VAL
2	B	109	VAL

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Mol	Chain	Res	Type
2	B	159	GLU
2	B	185	GLN
2	B	199	GLN
2	B	201	LEU
2	B	207	THR
2	B	208	ARG
2	B	212	ARG
2	B	229	VAL
2	B	243	ASP
2	B	247	ILE
2	B	253	LEU
2	B	281	LYS
2	B	288	TRP
2	B	297	SER
2	B	298	LYS
2	B	315	LEU
2	B	324	ARG
2	B	339	ILE
2	B	375	ASP
2	B	393	MET
2	B	394	GLU
2	B	395	LYS
2	B	400	LYS
2	B	406	LEU
2	B	419	LYS
2	B	426	LYS
2	B	440	LEU
2	B	441	VAL
2	B	446	VAL
2	B	454	ILE
2	B	470	GLU
2	B	481	ASN
2	B	484	LYS
2	B	495	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	21	HIS
2	A	59	GLN
2	A	286	HIS
2	A	341	ASN

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Mol	Chain	Res	Type
2	A	420	GLN
2	A	434	GLN
2	A	449	HIS
2	B	17	ASN
2	B	21	HIS
2	B	76	ASN
2	B	180	ASN
2	B	191	ASN
2	B	225	HIS
2	B	286	HIS
2	B	311	GLN
2	B	330	GLN
2	B	360	ASN
2	B	434	GLN
2	B	449	HIS
2	B	464	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	73/74 (98%)	21 (28%)	3 (4%)
1	D	73/74 (98%)	20 (27%)	13 (17%)
All	All	146/148 (98%)	41 (28%)	16 (10%)

All (41) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	8	U
1	C	10	G
1	C	12	U
1	C	14	A
1	C	15	G
1	C	16	C
1	C	17	U
1	C	18	G
1	C	20	U
1	C	20(A)	C
1	C	21	A
1	C	34	C
1	C	37	A
1	C	38	A

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Mol	Chain	Res	Type
1	C	45	G
1	C	46	G
1	C	48	C
1	C	49	G
1	C	54	U
1	C	59	G
1	C	60	U
1	D	8	U
1	D	10	G
1	D	16	C
1	D	17	U
1	D	18	G
1	D	20(A)	C
1	D	21	A
1	D	34	C
1	D	37	A
1	D	45	G
1	D	46	G
1	D	48	C
1	D	49	G
1	D	52	G
1	D	57	G
1	D	58	A
1	D	59	G
1	D	61	C
1	D	62	C
1	D	63	U

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	33	U
1	C	36	U
1	C	58	A
1	D	7	G
1	D	9	A
1	D	15	G
1	D	20	U
1	D	20(A)	C
1	D	33	U
1	D	36	U
1	D	45	G

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Mol	Chain	Res	Type
1	D	47	U
1	D	48	C
1	D	57	G
1	D	58	A
1	D	60	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	MSP	A	501	-	27,33,33	0.90	0	34,48,48	1.89	9 (26%)
3	MSP	B	1501	-	27,33,33	0.77	0	34,48,48	2.03	11 (32%)

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	MSP	A	501	-	1/1/11/15	0/22/62/62	0/3/3/3
3	MSP	B	1501	-	1/1/11/15	0/22/62/62	0/3/3/3

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	MSP	C5-C4-N9	4.92	107.18	101.25
3	B	1501	MSP	C5-C4-N9	4.68	106.89	101.25
3	B	1501	MSP	O2S-S1-O1S	-4.22	114.53	120.85
3	B	1501	MSP	O5'-C5'-C4'	4.21	115.07	107.57
3	A	501	MSP	O2S-S1-O1S	-3.73	115.27	120.85
3	B	1501	MSP	C2'-C1'-N9	-3.67	106.77	113.85
3	A	501	MSP	O5'-C5'-C4'	3.44	113.71	107.57
3	A	501	MSP	O5'-S1-N8	3.39	114.46	105.69
3	A	501	MSP	O1-C9-N8	3.36	129.09	122.98
3	B	1501	MSP	O1-C9-N8	3.18	128.75	122.98
3	B	1501	MSP	C5-C6-N6	-3.08	120.80	124.68
3	B	1501	MSP	O5'-S1-N8	2.87	113.12	105.69
3	A	501	MSP	C5-C6-N6	-2.84	121.11	124.68
3	B	1501	MSP	C5-C6-N1	2.61	121.57	116.08
3	A	501	MSP	O4'-C1'-C2'	-2.60	101.06	106.62
3	A	501	MSP	C5-C6-N1	2.60	121.54	116.08
3	B	1501	MSP	C3'-C2'-C1'	2.58	106.35	101.46
3	B	1501	MSP	O5'-S1-O1S	2.47	112.95	105.48
3	A	501	MSP	O2'-C2'-C1'	2.25	117.84	110.10
3	B	1501	MSP	O2'-C2'-C1'	2.01	117.02	110.10

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	501	MSP	C4
3	B	1501	MSP	C4

There are no torsion outliers.

There are no ring outliers.

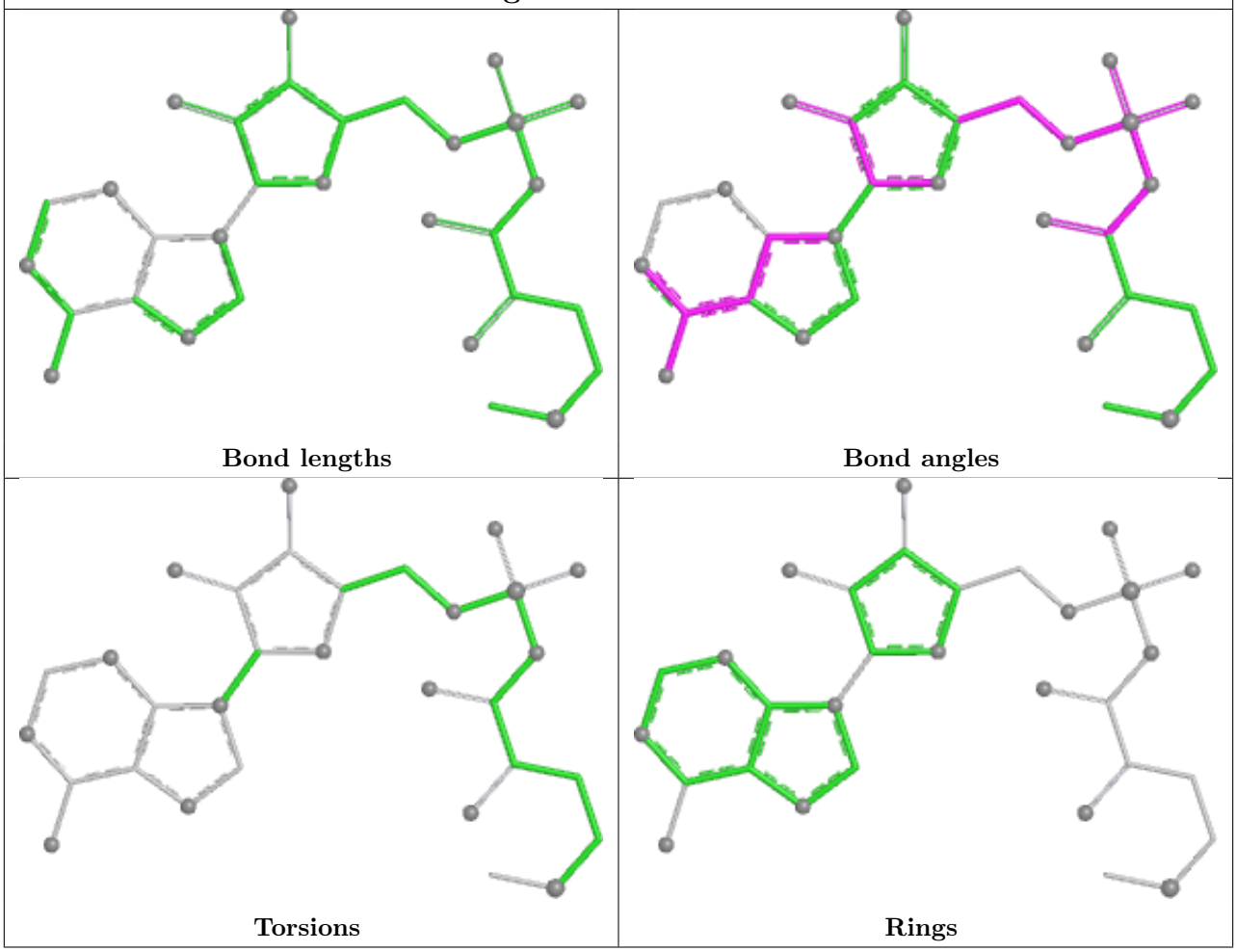
2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	MSP	6	0
3	B	1501	MSP	6	0

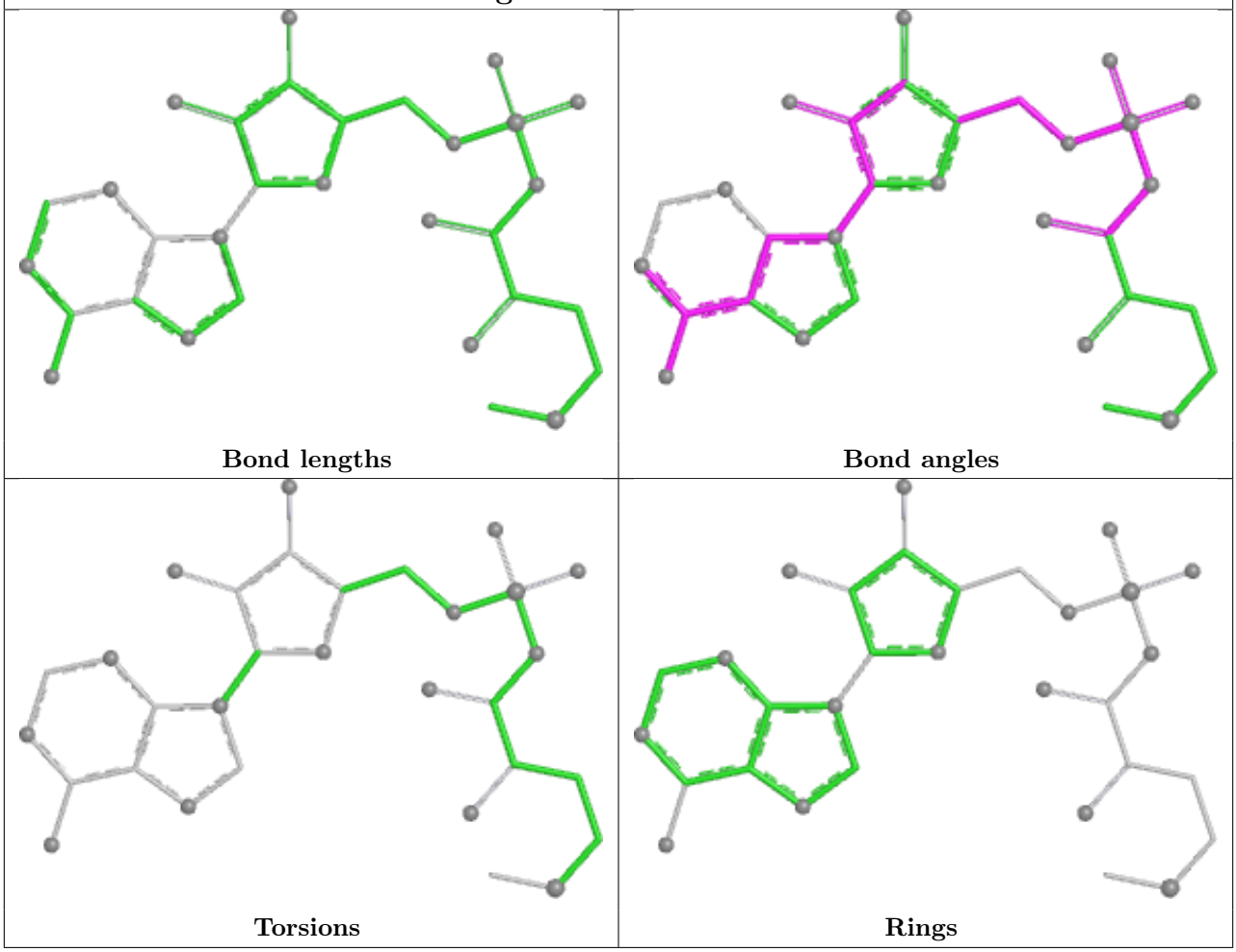
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand MSP A 501



Ligand MSP B 1501



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	C	74/74 (100%)	0.64	9 (12%)	4	3	44, 129, 161, 166	0
1	D	74/74 (100%)	0.48	8 (10%)	5	4	32, 97, 162, 170	0
2	A	465/497 (93%)	-0.14	6 (1%)	77	78	15, 36, 65, 91	0
2	B	465/497 (93%)	-0.20	7 (1%)	73	76	16, 31, 50, 85	0
All	All	1078/1142 (94%)	-0.07	30 (2%)	53	54	15, 36, 130, 170	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	45	G	7.8
1	D	56	C	7.6
1	D	20(A)	C	6.6
1	D	17	U	6.6
1	D	20	U	6.3
1	D	16	C	6.0
1	C	16	C	5.9
2	B	1	MET	5.6
2	B	160	PRO	5.5
1	C	47	U	5.0
2	A	158	LYS	4.7
1	D	19	G	4.4
1	C	64	C	4.2
1	C	17	U	4.1
1	C	65	C	4.1
2	B	159	GLU	4.0
1	C	20(A)	C	3.9
2	B	125	GLU	3.9
2	B	158	LYS	3.8
2	A	497	GLY	3.5
2	A	1	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	66	C	2.8
1	C	20	U	2.8
1	D	55	U	2.8
2	B	124	TYR	2.5
2	A	421	PRO	2.4
1	D	57	G	2.3
2	B	212	ARG	2.3
2	A	364	LYS	2.1
2	A	60	LYS	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

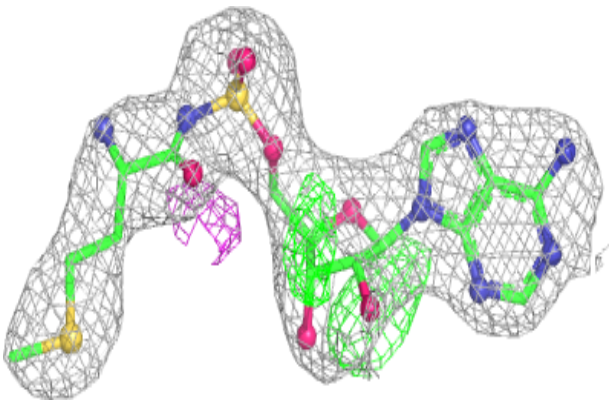
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

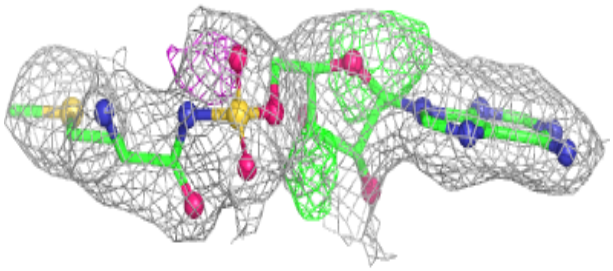
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MSP	A	501	31/31	0.95	0.17	24,41,45,49	0
3	MSP	B	1501	31/31	0.95	0.19	21,34,42,48	0

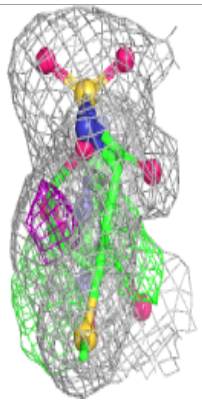
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around MSP A 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

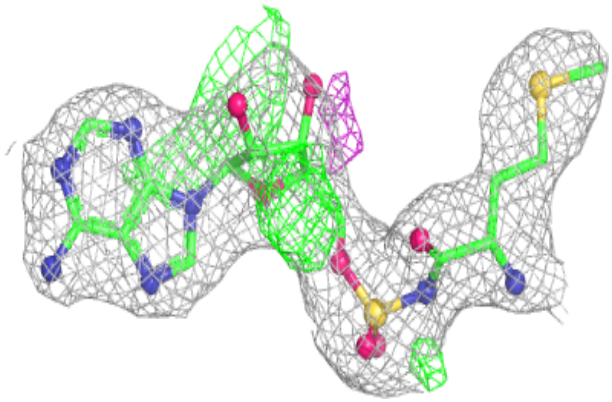


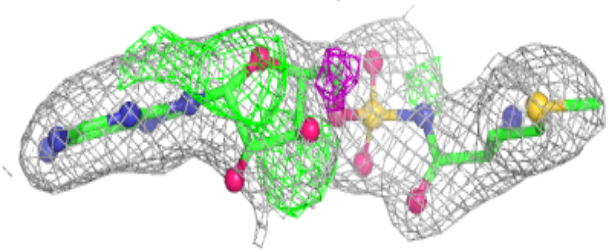


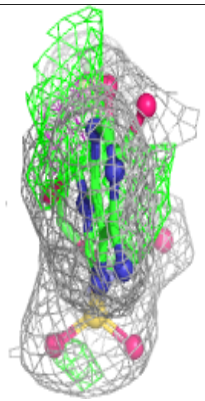


Electron density around MSP B 1501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.