



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:05 PM UTC

PDB ID : 2DEU / pdb_00002deu
Title : Cocrystal structure of an RNA sulfuration enzyme MnmA and tRNA-Glu in the adenylated intermediate state
Authors : Numata, T.; Ikeuchi, Y.; Fukai, S.; Suzuki, T.; Nureki, O.
Deposited on : 2006-02-17
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

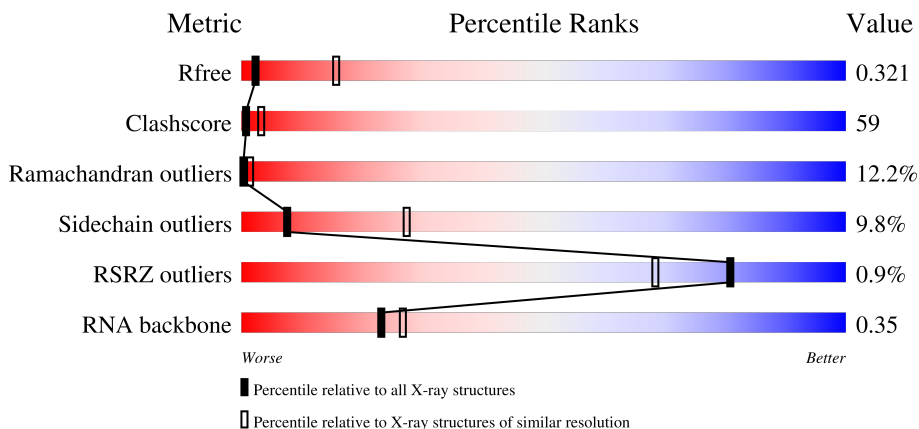
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)
RNA backbone	3983	1157 (3.80-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	C	76	28% 41% 18% 11% •
1	D	76	25% 43% 17% 12% •
2	A	380	23% 57% 15% • •
2	B	380	24% 53% 17% • •

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
4	SO4	B	5002	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8908 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 tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	74	Total	C	N	O	P	0	0	0
			1573	701	279	519	74			
1	D	74	Total	C	N	O	P	0	0	0
			1573	701	279	519	74			

- Molecule 2 is a protein called tRNA-specific 2-thiouridylase mnmA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	364	Total	C	N	O	S	0	0	0
			2854	1810	485	547	12			
2	B	364	Total	C	N	O	S	0	0	0
			2854	1810	485	547	12			

There are 24 discrepancies between the modelled and reference sequences:

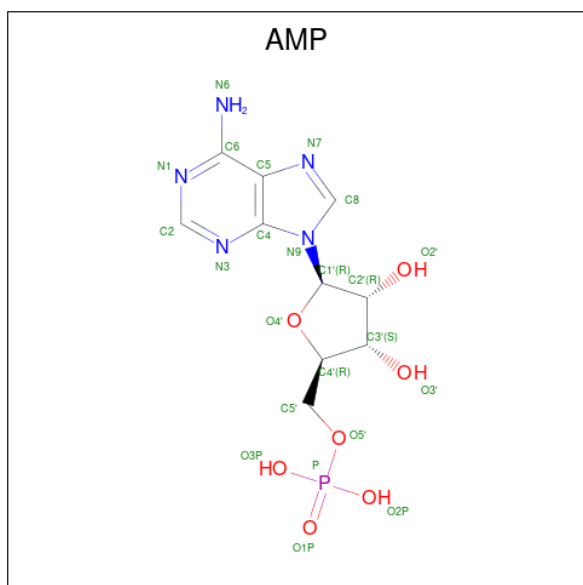
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP P25745
A	-10	ARG	-	expression tag	UNP P25745
A	-9	GLY	-	expression tag	UNP P25745
A	-8	SER	-	expression tag	UNP P25745
A	-7	HIS	-	expression tag	UNP P25745
A	-6	HIS	-	expression tag	UNP P25745
A	-5	HIS	-	expression tag	UNP P25745
A	-4	HIS	-	expression tag	UNP P25745
A	-3	HIS	-	expression tag	UNP P25745
A	-2	HIS	-	expression tag	UNP P25745
A	-1	GLY	-	expression tag	UNP P25745
A	0	SER	-	expression tag	UNP P25745
B	-11	MET	-	expression tag	UNP P25745
B	-10	ARG	-	expression tag	UNP P25745
B	-9	GLY	-	expression tag	UNP P25745
B	-8	SER	-	expression tag	UNP P25745
B	-7	HIS	-	expression tag	UNP P25745

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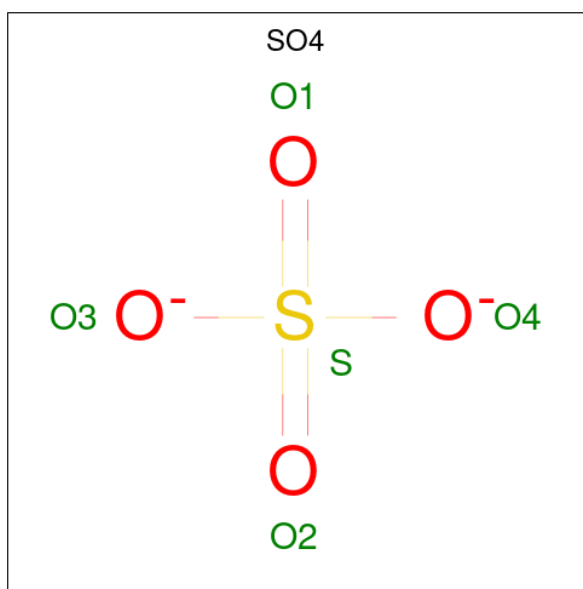
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP P25745
B	-5	HIS	-	expression tag	UNP P25745
B	-4	HIS	-	expression tag	UNP P25745
B	-3	HIS	-	expression tag	UNP P25745
B	-2	HIS	-	expression tag	UNP P25745
B	-1	GLY	-	expression tag	UNP P25745
B	0	SER	-	expression tag	UNP P25745

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
3	D	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).

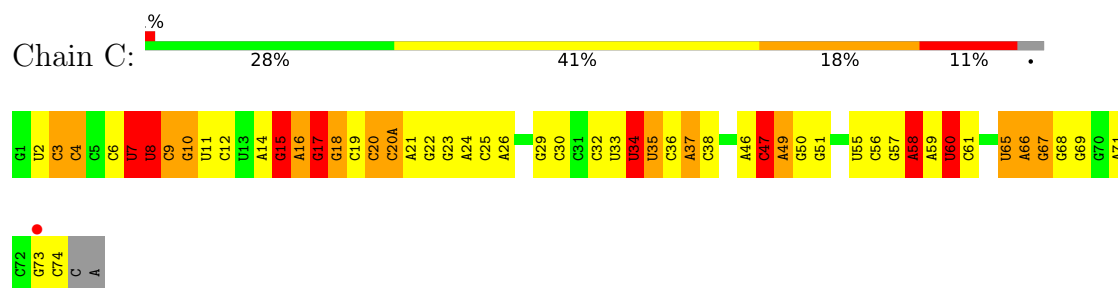


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

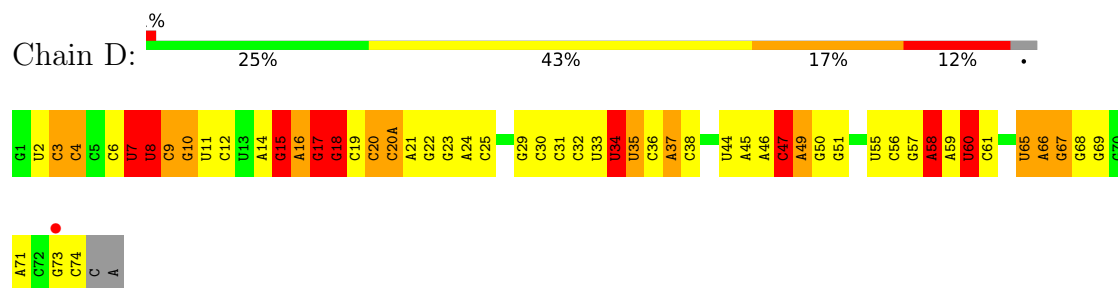
3 Residue-property plots [i](#)

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.

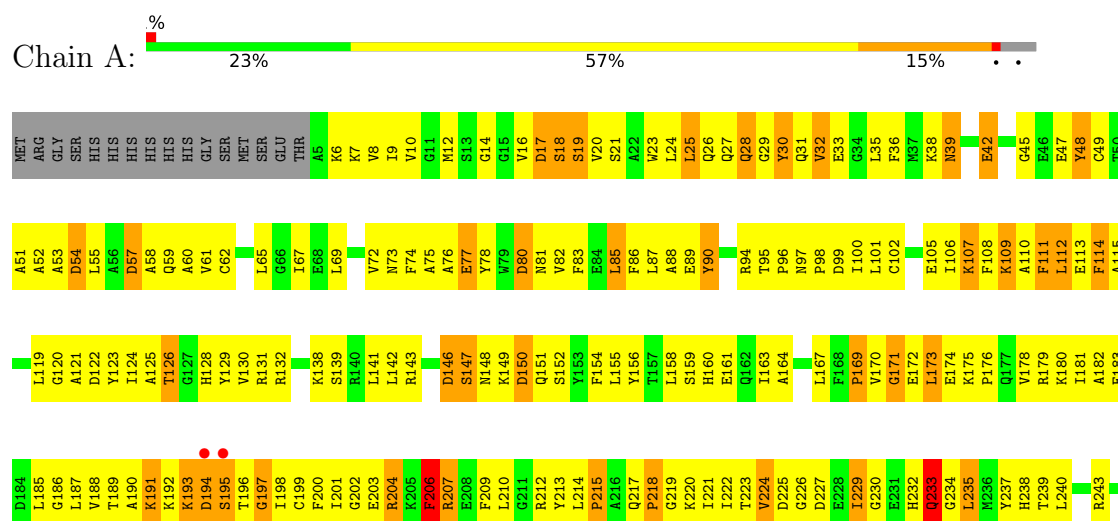
• Molecule 1: tRNA

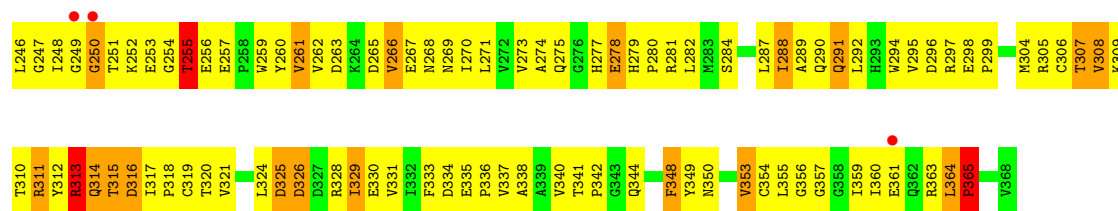


• Molecule 1: tRNA



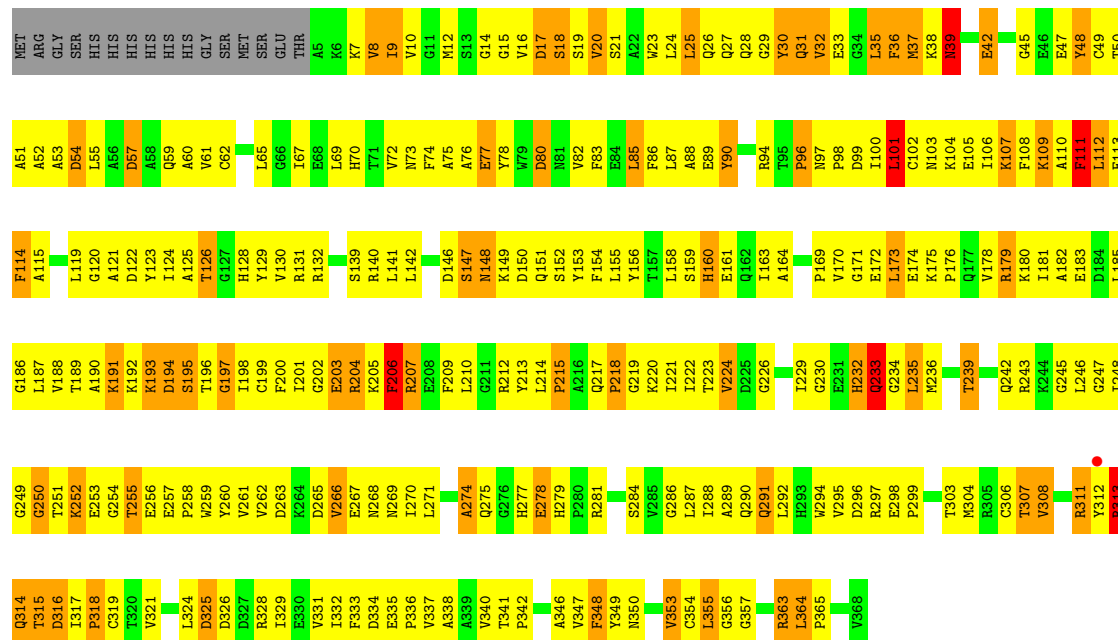
• Molecule 2: tRNA-specific 2-thiouridylase mnmA





• Molecule 2: tRNA-specific 2-thiouridylase mmmA

Chain B: 24% 53% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	238.06Å 102.13Å 108.16Å 90.00° 117.03° 90.00°	Depositor
Resolution (Å)	39.16 – 3.40 39.16 – 3.40	Depositor EDS
% Data completeness (in resolution range)	94.6 (39.16-3.40) 94.5 (39.16-3.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 3.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.281 , 0.318 0.260 , 0.321	Depositor DCC
R_{free} test set	1971 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	87.0	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 160.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.450 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8908	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AMP, SO4

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	0.61	0/1755	1.16	14/2731 (0.5%)
1	D	0.60	0/1755	1.15	12/2731 (0.4%)
2	A	0.51	0/2913	1.05	18/3941 (0.5%)
2	B	0.51	0/2913	1.04	15/3941 (0.4%)
All	All	0.55	0/9336	1.09	59/13344 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	3
1	D	0	4
All	All	0	7

There are no bond length outliers.

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	7	U	C2'-C3'-O3'	8.57	122.36	109.50
1	D	7	U	C2'-C3'-O3'	8.39	122.08	109.50
1	D	60	U	C4'-C3'-O3'	-8.31	100.54	113.00
1	C	60	U	C4'-C3'-O3'	-7.99	101.01	113.00
2	A	31	GLN	N-CA-C	-7.47	97.89	109.76
2	B	31	GLN	N-CA-C	-7.23	98.26	109.76
2	B	32	VAL	N-CA-C	7.19	118.72	107.28
2	A	32	VAL	N-CA-C	7.04	118.48	107.28
2	A	353	VAL	CB-CA-C	-6.92	102.09	111.63
1	C	34	U	C2'-C3'-O3'	6.74	123.81	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	47	C	C4'-C3'-O3'	-6.74	102.90	113.00
2	A	25	LEU	N-CA-C	-6.70	103.23	111.40
1	C	15	G	C2'-C3'-O3'	6.64	119.46	109.50
1	C	47	C	C4'-C3'-O3'	-6.63	103.05	113.00
1	C	17	G	C4'-C3'-O3'	-6.57	103.15	113.00
2	B	25	LEU	N-CA-C	-6.53	103.43	111.40
1	D	15	G	C2'-C3'-O3'	6.52	119.28	109.50
1	D	17	G	C4'-C3'-O3'	-6.52	103.23	113.00
2	B	364	LEU	CA-C-N	6.50	127.97	119.84
2	B	364	LEU	C-N-CA	6.50	127.97	119.84
2	A	224	VAL	N-CA-C	-6.50	104.86	112.98
1	D	60	U	N1-C1'-C2'	6.45	121.67	112.00
1	C	60	U	N1-C1'-C2'	6.37	121.56	112.00
1	C	47	C	N1-C1'-C2'	6.33	121.50	112.00
1	D	47	C	N1-C1'-C2'	6.29	121.43	112.00
2	A	57	ASP	N-CA-C	-6.26	104.53	111.36
2	B	57	ASP	N-CA-C	-6.22	104.58	111.36
1	D	34	U	C2'-C3'-O3'	6.21	123.02	113.70
1	D	58	A	C4'-C3'-O3'	-6.10	103.85	113.00
1	C	58	A	C4'-C3'-O3'	-6.06	103.91	113.00
1	C	18	G	N9-C1'-C2'	5.98	122.97	114.00
2	A	364	LEU	CA-C-N	5.93	127.25	119.84
2	A	364	LEU	C-N-CA	5.93	127.25	119.84
1	D	18	G	N9-C1'-C2'	5.89	122.83	114.00
1	C	8	U	C4'-C3'-O3'	-5.84	104.23	113.00
2	A	151	GLN	N-CA-C	5.71	119.84	112.41
2	B	308	VAL	N-CA-C	5.68	115.33	108.06
2	B	224	VAL	N-CA-C	-5.67	105.90	112.98
2	A	308	VAL	N-CA-C	5.67	115.31	108.06
2	B	101	LEU	N-CA-C	-5.61	106.79	113.97
2	A	101	LEU	N-CA-C	-5.59	106.82	113.97
2	A	338	ALA	N-CA-C	5.48	117.64	109.25
2	B	39	ASN	N-CA-C	5.44	119.90	112.88
2	B	338	ALA	N-CA-C	5.44	117.58	109.25
1	D	8	U	C4'-C3'-O3'	-5.43	104.85	113.00
2	A	14	GLY	N-CA-C	-5.34	106.85	115.08
2	A	359	ILE	N-CA-C	5.21	116.09	108.58
1	C	17	G	N9-C1'-C2'	5.20	119.79	112.00
2	A	311	ARG	N-CA-C	-5.17	99.79	110.80
2	B	353	VAL	N-CA-C	5.17	116.68	109.55
2	A	353	VAL	N-CA-C	5.14	116.64	109.55
1	C	58	A	N9-C1'-C2'	5.14	119.71	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	54	ASP	N-CA-C	-5.13	106.12	112.38
2	A	39	ASN	N-CA-C	5.13	120.18	112.94
1	D	58	A	N9-C1'-C2'	5.10	119.65	112.00
1	C	34	U	C4'-C3'-O3'	-5.09	105.37	113.00
2	A	126	THR	N-CA-C	-5.02	103.03	110.46
2	B	126	THR	N-CA-C	-5.02	103.04	110.46
2	B	311	ARG	N-CA-C	-5.01	100.14	110.80

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	17	G	Sidechain
1	C	47	C	Sidechain
1	C	60	U	Sidechain
1	D	17	G	Sidechain
1	D	18	G	Sidechain
1	D	47	C	Sidechain
1	D	60	U	Sidechain

5.2 Too-close contacts

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	1573	0	802	76	0
1	D	1573	0	802	77	0
2	A	2854	0	2799	399	0
2	B	2854	0	2799	409	0
3	C	22	0	12	3	0
3	D	22	0	12	4	0
4	A	5	0	0	1	0
4	B	5	0	0	2	0
All	All	8908	0	7226	946	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 59.

All (946) 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:21:A:H61	1:D:46:A:H2'	1.20	1.06
1:C:21:A:H61	1:C:46:A:H2'	1.15	1.04
2:A:196:THR:HG22	2:A:197:GLY:H	1.20	1.02
2:B:196:THR:HG22	2:B:197:GLY:H	1.26	0.99
1:D:56:C:H1'	2:A:185:LEU:HD23	1.45	0.98
2:B:19:SER:HB3	2:B:187:LEU:HD13	1.45	0.96
2:A:132:ARG:HE	2:A:164:ALA:HA	1.28	0.95
2:A:35:LEU:HD11	2:A:72:VAL:HG21	1.50	0.94
2:A:35:LEU:HD12	2:A:119:LEU:HD11	1.48	0.93
2:B:131:ARG:HH21	2:B:142:LEU:HD13	1.31	0.93
2:B:160:HIS:CD2	2:B:161:GLU:H	1.87	0.92
2:B:10:VAL:HG12	2:B:125:ALA:HB3	1.51	0.91
2:B:198:ILE:HD12	2:B:198:ILE:H	1.33	0.91
2:B:204:ARG:NH1	2:B:204:ARG:HB3	1.85	0.90
1:C:36:C:H4'	2:A:206:PHE:CE1	2.07	0.90
2:A:204:ARG:HB3	2:A:204:ARG:NH1	1.87	0.90
1:C:50:G:N2	1:C:65:U:H3	1.69	0.89
2:B:35:LEU:HD12	2:B:119:LEU:HD11	1.54	0.89
2:B:160:HIS:HD2	2:B:161:GLU:H	1.19	0.88
2:A:107:LYS:NZ	2:A:199:CYS:SG	2.47	0.88
2:B:85:LEU:HD12	2:B:85:LEU:H	1.39	0.87
1:D:50:G:N2	1:D:65:U:H3	1.72	0.87
2:B:38:LYS:C	2:B:39:ASN:HD22	1.83	0.86
2:A:160:HIS:HD2	2:A:161:GLU:H	1.23	0.86
2:A:298:GLU:HG3	2:A:299:PRO:HD2	1.58	0.86
2:B:97:ASN:O	2:B:100:ILE:HG22	1.75	0.86
2:B:10:VAL:HG23	2:B:12:MET:HE3	1.57	0.85
1:C:24:A:H2'	1:C:25:C:C6	2.11	0.85
2:B:73:ASN:HD21	2:B:75:ALA:HB3	1.40	0.84
2:B:262:VAL:HG13	2:B:281:ARG:O	1.77	0.84
2:A:198:ILE:HD12	2:A:198:ILE:H	1.43	0.84
2:A:160:HIS:CD2	2:A:161:GLU:H	1.96	0.84
2:B:8:VAL:HG23	2:B:31:GLN:O	1.78	0.84
2:B:89:GLU:HG2	2:B:94:ARG:NH2	1.92	0.84
2:B:296:ASP:OD1	2:B:298:GLU:HB2	1.77	0.84
2:B:132:ARG:HE	2:B:164:ALA:HA	1.42	0.83
2:B:232:HIS:CD2	2:B:271:LEU:HB2	2.14	0.83
2:A:111:PHE:CZ	2:A:124:ILE:HD11	2.12	0.83
2:B:284:SER:HB2	2:B:363:ARG:HH12	1.42	0.83
2:A:233:GLN:C	2:A:233:GLN:HE21	1.87	0.82
2:B:132:ARG:HD2	2:B:163:ILE:HG22	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:MET:HE1	2:B:111:PHE:HB2	1.59	0.82
2:B:70:HIS:ND1	2:B:119:LEU:HD22	1.94	0.82
2:A:10:VAL:HG12	2:A:125:ALA:HB3	1.60	0.81
2:A:61:VAL:HG13	2:A:187:LEU:HD22	1.61	0.81
2:A:296:ASP:OD1	2:A:298:GLU:HB2	1.81	0.81
1:D:24:A:H2'	1:D:25:C:C6	2.17	0.80
2:A:89:GLU:HG2	2:A:94:ARG:NH2	1.96	0.80
2:A:277:HIS:O	2:A:278:GLU:HG2	1.81	0.80
2:B:315:THR:O	2:B:317:ILE:HG23	1.82	0.80
2:A:196:THR:HG22	2:A:197:GLY:N	1.97	0.79
2:B:317:ILE:HD12	2:B:317:ILE:O	1.83	0.79
2:A:262:VAL:HG13	2:A:281:ARG:O	1.81	0.79
2:A:156:TYR:HB2	2:A:357:GLY:H	1.44	0.79
2:A:18:SER:O	2:A:21:SER:HB3	1.82	0.79
2:B:298:GLU:HG3	2:B:299:PRO:HD2	1.64	0.78
2:A:232:HIS:HD1	2:A:271:LEU:HD22	1.48	0.78
2:B:73:ASN:HD22	2:B:73:ASN:C	1.92	0.78
2:B:18:SER:O	2:B:21:SER:HB3	1.84	0.78
2:B:105:GLU:C	2:B:106:ILE:HD12	2.08	0.78
2:B:73:ASN:HD21	2:B:75:ALA:CB	1.98	0.77
2:B:156:TYR:HB2	2:B:357:GLY:H	1.48	0.76
2:A:35:LEU:HD23	2:A:36:PHE:N	2.00	0.76
2:A:95:THR:HG22	2:A:344:GLN:HE21	1.48	0.76
2:B:36:PHE:C	2:B:36:PHE:CD2	2.63	0.76
2:B:12:MET:HA	2:B:12:MET:HE2	1.67	0.75
1:C:21:A:N6	1:C:46:A:H2'	1.98	0.75
2:A:97:ASN:O	2:A:100:ILE:HG22	1.86	0.75
2:B:149:LYS:HZ2	2:B:175:LYS:HG2	1.52	0.75
1:D:25:C:H5'	2:B:256:GLU:O	1.87	0.75
2:A:315:THR:O	2:A:317:ILE:HG23	1.86	0.75
2:A:255:THR:H	2:A:275:GLN:HE22	1.32	0.75
2:A:111:PHE:CE1	2:A:124:ILE:HD11	2.22	0.74
2:A:107:LYS:HE2	2:A:200:PHE:CE2	2.23	0.74
2:B:36:PHE:C	2:B:36:PHE:HD2	1.95	0.73
2:A:312:TYR:CD1	2:A:313:ARG:N	2.56	0.73
2:A:204:ARG:HB3	2:A:204:ARG:HH11	1.51	0.73
2:A:24:LEU:HD11	2:A:173:LEU:HD11	1.69	0.73
2:A:221:ILE:HG12	2:A:271:LEU:HD23	1.70	0.73
2:B:222:ILE:HG22	2:B:223:THR:O	1.88	0.73
2:B:232:HIS:O	2:B:232:HIS:ND1	2.19	0.73
2:A:100:ILE:CG1	2:A:156:TYR:HE2	2.01	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:222:ILE:HG22	2:A:223:THR:O	1.89	0.72
2:B:223:THR:HG22	2:B:224:VAL:H	1.54	0.72
2:A:156:TYR:HB2	2:A:357:GLY:N	2.03	0.72
2:B:196:THR:HG22	2:B:197:GLY:N	2.04	0.72
2:A:262:VAL:HG11	2:A:281:ARG:HB3	1.70	0.72
2:B:232:HIS:HE1	2:B:235:LEU:HA	1.54	0.72
2:A:181:ILE:O	2:A:185:LEU:HG	1.89	0.72
2:A:100:ILE:HG12	2:A:156:TYR:HE2	1.55	0.72
2:B:102:CYS:SG	2:B:199:CYS:HB3	2.29	0.71
1:C:25:C:H5'	2:A:256:GLU:O	1.89	0.71
2:A:12:MET:HE2	2:A:12:MET:HA	1.72	0.71
2:A:317:ILE:O	2:A:317:ILE:HG13	1.88	0.71
1:D:20:C:H5''	1:D:20(A):C:OP1	1.90	0.71
2:A:266:VAL:HG23	2:A:267:GLU:H	1.55	0.71
2:B:223:THR:HG22	2:B:224:VAL:N	2.06	0.71
2:B:10:VAL:CG2	2:B:12:MET:HE3	2.20	0.71
2:B:204:ARG:HB3	2:B:204:ARG:HH11	1.56	0.70
2:A:130:VAL:HG22	2:A:131:ARG:N	2.05	0.70
2:A:314:GLN:HG2	2:A:315:THR:H	1.56	0.70
2:A:185:LEU:HD12	2:A:187:LEU:HD11	1.74	0.70
2:B:107:LYS:CE	2:B:199:CYS:SG	2.80	0.70
2:A:73:ASN:HD21	2:A:75:ALA:HB3	1.57	0.69
2:B:72:VAL:HG11	2:B:74:PHE:CE1	2.26	0.69
1:C:20:C:H5''	1:C:20(A):C:OP1	1.91	0.69
2:A:232:HIS:NE2	2:A:235:LEU:HD13	2.08	0.69
2:B:160:HIS:CD2	2:B:161:GLU:N	2.60	0.69
2:B:20:VAL:HG23	2:B:182:ALA:HB2	1.73	0.69
2:A:130:VAL:HG21	2:A:141:LEU:HD11	1.75	0.68
2:A:223:THR:HG22	2:A:224:VAL:H	1.57	0.68
2:A:102:CYS:SG	2:A:199:CYS:HB3	2.33	0.68
2:B:279:HIS:CD2	2:B:281:ARG:H	2.12	0.68
2:B:102:CYS:SG	2:B:107:LYS:NZ	2.62	0.68
2:A:260:TYR:OH	2:A:277:HIS:HB2	1.93	0.68
2:A:83:PHE:O	2:A:86:PHE:HB3	1.94	0.68
2:B:8:VAL:HG21	2:B:30:TYR:HB3	1.76	0.68
2:B:156:TYR:HB2	2:B:357:GLY:N	2.07	0.68
2:B:83:PHE:O	2:B:86:PHE:HB3	1.93	0.68
2:B:107:LYS:HE2	2:B:199:CYS:SG	2.34	0.68
2:B:287:LEU:C	2:B:287:LEU:HD12	2.19	0.68
2:A:129:TYR:OH	2:A:146:ASP:HB2	1.95	0.67
2:B:232:HIS:ND1	2:B:234:GLY:O	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:36:PHE:CD2	2:A:55:LEU:HD13	2.29	0.67
1:D:21:A:N6	1:D:46:A:H2'	2.04	0.67
2:A:39:ASN:HB2	2:A:200:PHE:CD1	2.30	0.67
2:A:196:THR:CG2	2:A:197:GLY:H	2.03	0.67
2:A:25:LEU:HD23	2:A:28:GLN:NE2	2.09	0.67
2:A:232:HIS:ND1	2:A:271:LEU:HD22	2.10	0.67
2:A:265:ASP:HB2	2:A:270:ILE:HB	1.76	0.67
2:A:78:TYR:HA	2:A:106:ILE:HD11	1.77	0.67
2:A:255:THR:HB	2:A:257:GLU:HG3	1.76	0.67
2:B:221:ILE:HG12	2:B:271:LEU:HD23	1.75	0.67
2:A:213:TYR:O	2:A:214:LEU:HD23	1.94	0.66
2:B:102:CYS:HG	2:B:199:CYS:CB	2.08	0.66
2:B:103:ASN:OD1	2:B:128:HIS:HE1	1.77	0.66
2:B:9:ILE:HA	2:B:33:GLU:O	1.96	0.66
2:B:35:LEU:HD23	2:B:36:PHE:N	2.11	0.66
2:B:270:ILE:HG22	2:B:271:LEU:H	1.61	0.65
2:A:156:TYR:HD1	2:A:357:GLY:H	1.42	0.65
1:C:9:C:H5'	1:C:10:G:OP2	1.96	0.65
2:B:102:CYS:HG	2:B:199:CYS:HB3	1.60	0.65
1:C:36:C:H4'	2:A:206:PHE:HE1	1.60	0.65
2:B:61:VAL:HG13	2:B:187:LEU:HD22	1.78	0.65
2:A:23:TRP:HB2	2:A:65:LEU:HD21	1.77	0.65
2:B:284:SER:HB2	2:B:363:ARG:NH1	2.11	0.65
2:B:130:VAL:HG22	2:B:131:ARG:N	2.11	0.65
2:A:279:HIS:ND1	2:A:280:PRO:HD2	2.12	0.65
2:A:270:ILE:HG22	2:A:271:LEU:H	1.63	0.64
2:A:288:ILE:HD12	2:A:330:GLU:HA	1.80	0.64
2:B:85:LEU:HD12	2:B:85:LEU:N	2.10	0.64
2:B:314:GLN:HG2	2:B:315:THR:H	1.62	0.64
2:A:39:ASN:HB2	2:A:200:PHE:HD1	1.62	0.64
2:A:265:ASP:OD2	2:A:270:ILE:HD12	1.96	0.64
2:A:8:VAL:HG21	2:A:30:TYR:CD2	2.32	0.64
2:A:73:ASN:HD21	2:A:75:ALA:CB	2.10	0.64
2:B:35:LEU:HD23	2:B:35:LEU:C	2.23	0.64
2:B:261:VAL:HG12	2:B:262:VAL:N	2.13	0.64
2:A:81:ASN:HB3	2:A:105:GLU:OE1	1.98	0.64
2:A:83:PHE:CE2	2:A:87:LEU:HD11	2.33	0.64
2:B:32:VAL:O	2:B:67:ILE:HG23	1.97	0.64
2:A:160:HIS:CD2	2:A:161:GLU:N	2.65	0.64
2:A:314:GLN:HG2	2:A:315:THR:N	2.12	0.64
2:A:353:VAL:HG12	2:A:354:CYS:N	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:VAL:CG2	2:B:30:TYR:HB3	2.27	0.64
1:C:56:C:H1'	2:B:185:LEU:HD23	1.80	0.64
2:A:190:ALA:O	2:A:191:LYS:HB2	1.97	0.64
2:A:287:LEU:HD23	2:A:333:PHE:CZ	2.32	0.63
2:A:331:VAL:HG21	2:A:348:PHE:HE2	1.63	0.63
2:B:199:CYS:O	2:B:200:PHE:HB2	1.98	0.63
2:B:83:PHE:HE1	2:B:87:LEU:HD11	1.63	0.63
1:C:24:A:H2'	1:C:25:C:H6	1.61	0.63
1:D:36:C:H4'	2:B:206:PHE:CE1	2.33	0.63
2:B:20:VAL:HG11	2:B:178:VAL:HG13	1.81	0.63
2:B:73:ASN:HD22	2:B:75:ALA:H	1.46	0.63
1:C:11:U:H2'	1:C:12:C:C6	2.34	0.63
2:A:290:GLN:O	2:A:292:LEU:HD23	1.99	0.63
2:B:348:PHE:N	2:B:348:PHE:CD1	2.67	0.63
2:A:42:GLU:CD	2:A:42:GLU:H	2.07	0.63
2:A:146:ASP:OD1	2:A:174:GLU:HB3	1.99	0.63
2:B:85:LEU:H	2:B:85:LEU:CD1	2.10	0.63
2:B:111:PHE:CD1	2:B:124:ILE:HD11	2.34	0.63
1:C:36:C:H4'	2:A:206:PHE:CD1	2.34	0.62
2:B:90:TYR:CE2	2:B:96:PRO:HD2	2.34	0.62
2:B:290:GLN:O	2:B:292:LEU:N	2.32	0.62
2:B:292:LEU:HD21	2:B:329:ILE:CD1	2.29	0.62
1:D:56:C:H1'	2:A:185:LEU:CD2	2.25	0.62
2:A:90:TYR:CE2	2:A:96:PRO:HD2	2.34	0.62
2:A:9:ILE:HA	2:A:33:GLU:O	1.99	0.62
2:B:100:ILE:HG12	2:B:156:TYR:HE2	1.63	0.62
2:B:206:PHE:O	2:B:209:PHE:N	2.33	0.62
2:A:17:ASP:HB2	4:A:5001:SO4:O3	2.00	0.62
2:B:36:PHE:CD1	2:B:55:LEU:HD12	2.34	0.62
2:B:198:ILE:H	2:B:198:ILE:CD1	2.11	0.62
2:A:288:ILE:HG13	2:A:329:ILE:O	1.99	0.62
2:B:313:ARG:HH11	2:B:313:ARG:CB	2.12	0.62
2:B:108:PHE:CG	2:B:158:LEU:HD21	2.35	0.62
2:A:32:VAL:O	2:A:67:ILE:HG23	2.00	0.62
2:A:290:GLN:O	2:A:292:LEU:N	2.33	0.61
2:A:308:VAL:O	2:A:317:ILE:HG12	2.00	0.61
2:A:6:LYS:HB3	2:A:122:ASP:OD2	2.00	0.61
2:A:73:ASN:C	2:A:73:ASN:HD22	2.08	0.61
2:A:130:VAL:HG22	2:A:131:ARG:H	1.65	0.61
2:A:288:ILE:CD1	2:A:330:GLU:HA	2.30	0.61
2:B:35:LEU:HD11	2:B:72:VAL:HG21	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:PHE:CE1	2:B:55:LEU:HA	2.35	0.61
2:B:37:MET:CE	2:B:111:PHE:HB2	2.29	0.61
2:A:265:ASP:CG	2:A:270:ILE:HD12	2.24	0.61
2:B:36:PHE:HE1	2:B:55:LEU:HA	1.64	0.61
2:A:199:CYS:O	2:A:200:PHE:HB2	2.00	0.61
2:A:284:SER:O	2:A:336:PRO:HA	2.01	0.61
2:A:317:ILE:HD12	2:A:337:VAL:HG21	1.81	0.61
2:B:284:SER:O	2:B:336:PRO:HA	2.00	0.61
2:B:265:ASP:OD2	2:B:270:ILE:HD12	2.00	0.61
2:A:141:LEU:HB2	2:A:163:ILE:CD1	2.31	0.61
2:B:261:VAL:CG1	2:B:262:VAL:N	2.64	0.61
2:B:149:LYS:NZ	2:B:179:ARG:HH12	1.98	0.61
2:A:106:ILE:O	2:A:108:PHE:N	2.34	0.61
2:A:333:PHE:HE2	2:A:340:VAL:HG21	1.66	0.61
2:B:159:SER:HB2	2:B:297:ARG:HG3	1.81	0.60
2:B:270:ILE:HG22	2:B:271:LEU:N	2.16	0.60
2:A:19:SER:HB3	2:A:187:LEU:HD13	1.83	0.60
2:B:204:ARG:HB3	2:B:204:ARG:CZ	2.31	0.60
2:A:257:GLU:HB2	2:A:275:GLN:HG3	1.83	0.60
1:C:58:A:O2'	1:C:60:U:H5	1.84	0.60
2:A:206:PHE:O	2:A:209:PHE:N	2.33	0.60
2:B:106:ILE:O	2:B:108:PHE:N	2.34	0.60
2:A:10:VAL:HG23	2:A:12:MET:HE3	1.82	0.60
2:B:39:ASN:HD22	2:B:39:ASN:N	1.99	0.60
2:B:350:ASN:CB	2:B:355:LEU:HD21	2.32	0.60
2:A:261:VAL:CG1	2:A:262:VAL:N	2.64	0.60
2:B:214:LEU:HB3	2:B:215:PRO:HD2	1.84	0.59
2:B:219:GLY:C	2:B:232:HIS:HB3	2.27	0.59
2:B:142:LEU:O	2:B:142:LEU:HD12	2.01	0.59
2:B:23:TRP:CE2	2:B:185:LEU:HD21	2.37	0.59
2:B:218:PRO:HA	2:B:234:GLY:H	1.65	0.59
2:B:232:HIS:O	2:B:233:GLN:C	2.46	0.59
2:A:149:LYS:HZ3	2:A:175:LYS:HG2	1.67	0.59
2:A:131:ARG:HB2	2:A:142:LEU:CD1	2.32	0.59
2:B:312:TYR:CD1	2:B:313:ARG:N	2.71	0.59
1:D:9:C:H5'	1:D:10:G:OP2	2.03	0.59
2:A:246:LEU:O	2:A:248:ILE:N	2.30	0.59
2:B:106:ILE:HG22	2:B:107:LYS:N	2.18	0.59
2:A:193:LYS:O	2:A:195:SER:N	2.36	0.59
2:B:146:ASP:OD1	2:B:174:GLU:HB3	2.02	0.59
2:B:7:LYS:HB3	2:B:121:ALA:HA	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:174:GLU:C	2:A:176:PRO:HD2	2.28	0.58
2:B:17:ASP:OD2	2:B:175:LYS:NZ	2.36	0.58
2:B:314:GLN:O	2:B:315:THR:HG23	2.03	0.58
2:A:349:TYR:CE2	2:A:354:CYS:HB2	2.38	0.58
2:B:193:LYS:O	2:B:195:SER:N	2.36	0.58
1:C:20:C:H4'	1:C:20(A):C:O5'	2.04	0.58
1:D:7:U:O2'	1:D:8:U:OP1	2.22	0.58
2:A:232:HIS:O	2:A:233:GLN:C	2.45	0.58
2:A:287:LEU:HD23	2:A:333:PHE:HZ	1.68	0.58
2:A:38:LYS:C	2:A:39:ASN:HD22	2.12	0.58
2:A:42:GLU:CD	2:A:42:GLU:N	2.61	0.58
2:A:237:TYR:C	2:A:238:HIS:HD2	2.12	0.58
2:B:77:GLU:HA	2:B:80:ASP:HB2	1.86	0.58
2:B:350:ASN:HB2	2:B:355:LEU:HD21	1.85	0.58
2:B:159:SER:O	2:B:163:ILE:HG13	2.04	0.58
1:D:59:A:H8	1:D:59:A:OP1	1.86	0.58
2:A:287:LEU:O	2:A:288:ILE:HD12	2.03	0.58
2:A:292:LEU:HD11	2:A:329:ILE:HG12	1.84	0.58
2:B:288:ILE:HG23	2:B:329:ILE:O	2.03	0.58
2:B:288:ILE:HD13	2:B:324:LEU:CD2	2.34	0.58
1:D:11:U:H2'	1:D:12:C:C6	2.38	0.58
2:A:142:LEU:HD12	2:A:142:LEU:O	2.04	0.58
2:B:286:GLY:HA3	2:B:364:LEU:HD12	1.86	0.58
1:D:20:C:H4'	1:D:20(A):C:O5'	2.03	0.57
2:A:21:SER:OG	2:A:169:PRO:HG3	2.04	0.57
2:A:35:LEU:HD23	2:A:35:LEU:C	2.29	0.57
2:B:156:TYR:HD1	2:B:357:GLY:H	1.49	0.57
2:B:257:GLU:HB2	2:B:275:GLN:HG2	1.84	0.57
2:B:292:LEU:HD21	2:B:329:ILE:HD11	1.85	0.57
2:A:317:ILE:HD12	2:A:337:VAL:CG2	2.35	0.57
2:B:232:HIS:CE1	2:B:235:LEU:HD13	2.39	0.57
2:B:267:GLU:C	2:B:269:ASN:H	2.11	0.57
2:B:314:GLN:HG2	2:B:315:THR:N	2.17	0.57
2:A:267:GLU:C	2:A:269:ASN:H	2.11	0.57
2:A:149:LYS:HD3	2:A:175:LYS:HG2	1.85	0.57
2:B:190:ALA:O	2:B:191:LYS:HB2	2.04	0.57
2:B:235:LEU:HD12	2:B:235:LEU:O	2.04	0.57
2:A:8:VAL:CG2	2:A:30:TYR:HD2	2.17	0.57
2:A:61:VAL:O	2:A:65:LEU:HD12	2.03	0.57
2:B:48:TYR:O	2:B:49:CYS:C	2.47	0.57
2:A:262:VAL:CG1	2:A:281:ARG:HB3	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:333:PHE:CE2	2:A:340:VAL:HG21	2.40	0.57
2:B:156:TYR:HB2	2:B:356:GLY:HA2	1.86	0.57
1:D:58:A:O2'	1:D:60:U:H5	1.87	0.57
2:A:180:LYS:O	2:A:183:GLU:N	2.37	0.57
1:C:7:U:O2'	1:C:8:U:OP1	2.22	0.56
2:A:218:PRO:HA	2:A:234:GLY:H	1.69	0.56
2:A:233:GLN:C	2:A:233:GLN:NE2	2.59	0.56
2:B:7:LYS:HE2	2:B:33:GLU:OE1	2.05	0.56
2:B:232:HIS:CE1	2:B:234:GLY:O	2.59	0.56
2:B:265:ASP:HB2	2:B:270:ILE:HB	1.87	0.56
2:B:286:GLY:N	2:B:333:PHE:CD2	2.73	0.56
2:B:355:LEU:HD23	2:B:355:LEU:N	2.20	0.56
1:C:7:U:N3	1:C:49:A:N7	2.53	0.56
2:A:156:TYR:HB2	2:A:356:GLY:HA2	1.86	0.56
2:A:156:TYR:HD1	2:A:357:GLY:N	2.04	0.56
2:A:146:ASP:O	2:A:147:SER:C	2.49	0.56
2:B:298:GLU:CG	2:B:299:PRO:HD2	2.34	0.56
1:D:7:U:N3	1:D:49:A:N7	2.53	0.56
2:A:9:ILE:HD13	2:A:119:LEU:CD1	2.36	0.56
2:A:48:TYR:O	2:A:49:CYS:C	2.48	0.56
2:B:198:ILE:HB	2:B:201:ILE:HB	1.86	0.56
2:A:232:HIS:CE1	2:A:235:LEU:HA	2.40	0.56
2:B:100:ILE:HD11	2:B:156:TYR:CD2	2.41	0.56
2:B:259:TRP:CE3	2:B:274:ALA:O	2.59	0.56
2:A:10:VAL:CG2	2:A:12:MET:HE3	2.36	0.56
2:A:141:LEU:HD12	2:A:142:LEU:H	1.70	0.56
1:C:20:C:O2	1:C:21:A:H1'	2.06	0.55
2:A:232:HIS:CE1	2:A:235:LEU:HD13	2.40	0.55
2:B:15:GLY:HA3	4:B:5002:SO4:O2	2.06	0.55
1:D:35:U:H6	1:D:35:U:H5'	1.70	0.55
2:A:198:ILE:HB	2:A:201:ILE:HB	1.88	0.55
2:A:223:THR:HG22	2:A:224:VAL:N	2.22	0.55
2:A:73:ASN:HD22	2:A:75:ALA:H	1.53	0.55
2:B:36:PHE:HD2	2:B:36:PHE:O	1.89	0.55
1:C:59:A:H8	1:C:59:A:OP1	1.90	0.55
1:D:50:G:H2'	1:D:51:G:H8	1.71	0.55
2:B:220:LYS:C	2:B:232:HIS:HB2	2.31	0.55
2:A:237:TYR:C	2:A:238:HIS:CD2	2.85	0.55
1:C:50:G:N2	1:C:65:U:N3	2.49	0.55
2:A:262:VAL:HG22	2:A:282:LEU:HD13	1.88	0.55
2:A:290:GLN:O	2:A:291:GLN:C	2.50	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:MET:HE2	2:B:12:MET:CA	2.36	0.55
2:B:239:THR:HG22	2:B:242:GLN:OE1	2.06	0.55
2:B:246:LEU:O	2:B:248:ILE:N	2.29	0.55
2:B:290:GLN:O	2:B:291:GLN:C	2.49	0.55
2:A:309:LYS:HE3	2:A:316:ASP:OD1	2.07	0.55
2:B:37:MET:HB3	2:B:39:ASN:HD21	1.72	0.55
2:B:353:VAL:HG12	2:B:355:LEU:HD23	1.89	0.55
2:A:295:VAL:HG13	2:A:296:ASP:N	2.21	0.55
2:B:130:VAL:HG21	2:B:141:LEU:HD11	1.89	0.55
2:B:146:ASP:O	2:B:147:SER:C	2.50	0.55
2:B:180:LYS:O	2:B:183:GLU:N	2.40	0.55
2:B:213:TYR:O	2:B:214:LEU:HD23	2.07	0.55
1:C:58:A:O2'	1:C:60:U:C5	2.59	0.54
2:A:97:ASN:O	2:A:98:PRO:C	2.50	0.54
2:A:170:VAL:C	2:A:172:GLU:H	2.14	0.54
2:B:306:CYS:HB2	2:B:349:TYR:O	2.07	0.54
1:D:20:C:O2	1:D:21:A:H1'	2.07	0.54
2:A:122:ASP:O	2:A:123:TYR:CD2	2.60	0.54
1:C:55:U:H5''	1:C:55:U:H6	1.72	0.54
2:A:183:GLU:OE2	2:A:191:LYS:HE3	2.06	0.54
2:A:255:THR:N	2:A:275:GLN:HE22	2.04	0.54
2:B:170:VAL:C	2:B:172:GLU:H	2.16	0.54
2:B:265:ASP:CG	2:B:270:ILE:HD12	2.33	0.54
2:A:270:ILE:HG22	2:A:271:LEU:N	2.21	0.54
2:B:260:TYR:OH	2:B:277:HIS:HB2	2.08	0.54
2:A:77:GLU:HA	2:A:80:ASP:HB2	1.88	0.54
2:A:82:VAL:HG12	2:A:83:PHE:N	2.23	0.54
2:A:214:LEU:HB3	2:A:215:PRO:HD2	1.88	0.54
2:B:73:ASN:C	2:B:73:ASN:ND2	2.63	0.54
2:A:74:PHE:O	2:A:77:GLU:HG2	2.08	0.54
2:A:156:TYR:CD1	2:A:357:GLY:N	2.76	0.54
2:A:159:SER:HB3	2:A:297:ARG:CZ	2.38	0.54
2:A:288:ILE:HA	2:A:329:ILE:O	2.07	0.54
2:A:304:MET:HB3	2:A:321:VAL:HB	1.90	0.54
2:B:59:GLN:O	2:B:62:CYS:N	2.41	0.54
2:B:78:TYR:HE1	2:B:82:VAL:HG11	1.73	0.54
2:B:89:GLU:CG	2:B:94:ARG:NH2	2.70	0.54
2:B:73:ASN:ND2	2:B:75:ALA:H	2.05	0.54
1:C:15:G:O2'	1:C:16:A:OP1	2.26	0.53
2:A:307:THR:HG23	2:A:349:TYR:O	2.08	0.53
2:B:38:LYS:C	2:B:39:ASN:ND2	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:194:ASP:O	2:A:195:SER:CB	2.56	0.53
2:B:217:GLN:O	2:B:217:GLN:HG2	2.08	0.53
2:A:240:LEU:HA	2:A:261:VAL:HG12	1.90	0.53
2:A:342:PRO:HA	2:A:360:ILE:HG22	1.90	0.53
2:A:238:HIS:CD2	2:A:238:HIS:N	2.77	0.53
2:B:147:SER:O	2:B:148:ASN:C	2.52	0.53
2:B:217:GLN:N	2:B:217:GLN:OE1	2.41	0.53
1:D:23:G:O2'	1:D:24:A:H5'	2.09	0.53
2:A:7:LYS:HB3	2:A:121:ALA:HA	1.90	0.53
2:A:132:ARG:NE	2:A:164:ALA:HA	2.11	0.53
2:A:185:LEU:HD12	2:A:187:LEU:CD1	2.37	0.53
2:B:194:ASP:O	2:B:195:SER:HB3	2.09	0.53
2:B:308:VAL:O	2:B:317:ILE:HG13	2.09	0.53
1:C:35:U:H6	1:C:35:U:H5'	1.73	0.53
2:A:232:HIS:NE2	2:A:235:LEU:HB2	2.23	0.53
2:A:59:GLN:O	2:A:62:CYS:N	2.42	0.53
2:B:100:ILE:CG1	2:B:156:TYR:HE2	2.21	0.53
1:C:17:G:N2	1:C:55:U:O2	2.42	0.53
3:D:134:AMP:H5'2	4:B:5002:SO4:O1	2.09	0.53
2:A:17:ASP:O	2:A:18:SER:C	2.52	0.53
2:A:25:LEU:O	2:A:26:GLN:C	2.52	0.53
2:A:221:ILE:HG13	2:A:232:HIS:N	2.23	0.53
2:B:59:GLN:O	2:B:61:VAL:N	2.42	0.53
2:B:295:VAL:HG13	2:B:296:ASP:N	2.24	0.53
1:C:50:G:H2'	1:C:51:G:H8	1.74	0.52
2:A:61:VAL:HG12	2:A:65:LEU:CD1	2.39	0.52
2:A:204:ARG:HB3	2:A:204:ARG:CZ	2.39	0.52
2:B:221:ILE:CD1	2:B:271:LEU:HD23	2.39	0.52
2:B:288:ILE:HA	2:B:329:ILE:O	2.09	0.52
1:D:50:G:N2	1:D:65:U:N3	2.51	0.52
2:A:169:PRO:HG2	2:A:170:VAL:H	1.73	0.52
2:A:331:VAL:HG21	2:A:348:PHE:CE2	2.42	0.52
2:B:17:ASP:O	2:B:18:SER:C	2.52	0.52
2:A:9:ILE:HD13	2:A:119:LEU:HD12	1.91	0.52
1:D:58:A:O2'	1:D:60:U:C5	2.62	0.52
1:D:58:A:HO2'	1:D:60:U:H5	1.57	0.52
2:A:147:SER:O	2:A:148:ASN:C	2.52	0.52
2:B:48:TYR:O	2:B:51:ALA:N	2.42	0.52
2:B:111:PHE:C	2:B:111:PHE:CD2	2.87	0.52
2:B:221:ILE:HG13	2:B:232:HIS:N	2.24	0.52
2:A:170:VAL:C	2:A:172:GLU:N	2.65	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:217:GLN:OE1	2:A:217:GLN:N	2.41	0.52
2:B:97:ASN:O	2:B:98:PRO:C	2.52	0.52
2:B:196:THR:N	2:B:203:GLU:OE2	2.43	0.52
2:A:219:GLY:C	2:A:232:HIS:HB3	2.35	0.52
2:A:255:THR:C	2:A:257:GLU:H	2.18	0.52
1:D:67:G:H21	1:D:68:G:H1'	1.74	0.52
2:A:20:VAL:CG2	2:A:182:ALA:HB2	2.39	0.52
2:A:218:PRO:HA	2:A:233:GLN:HA	1.91	0.52
2:A:304:MET:HG3	2:A:305:ARG:H	1.75	0.52
2:B:102:CYS:O	2:B:107:LYS:HG3	2.10	0.52
1:D:10:G:H2'	1:D:11:U:C6	2.45	0.52
2:A:74:PHE:HE1	2:A:111:PHE:HA	1.73	0.52
2:B:39:ASN:N	2:B:39:ASN:ND2	2.56	0.52
2:B:176:PRO:O	2:B:180:LYS:HG2	2.10	0.52
2:B:194:ASP:O	2:B:195:SER:CB	2.58	0.52
2:B:25:LEU:O	2:B:26:GLN:C	2.52	0.51
2:B:348:PHE:N	2:B:348:PHE:HD1	2.07	0.51
2:A:39:ASN:HA	2:A:75:ALA:HB2	1.92	0.51
2:A:232:HIS:O	2:A:234:GLY:O	2.28	0.51
2:B:9:ILE:HG21	2:B:119:LEU:HD13	1.92	0.51
2:B:72:VAL:HG12	2:B:73:ASN:N	2.25	0.51
2:B:106:ILE:HD12	2:B:106:ILE:N	2.25	0.51
2:B:363:ARG:NH1	2:B:363:ARG:HB2	2.25	0.51
1:D:55:U:H5''	1:D:55:U:H6	1.75	0.51
2:A:52:ALA:O	2:A:55:LEU:HB3	2.11	0.51
2:A:173:LEU:HD13	2:A:178:VAL:HG22	1.92	0.51
2:A:180:LYS:O	2:A:181:ILE:C	2.52	0.51
2:B:108:PHE:CB	2:B:158:LEU:HD21	2.40	0.51
2:A:48:TYR:O	2:A:51:ALA:N	2.43	0.51
2:B:106:ILE:HA	2:B:110:ALA:HB3	1.92	0.51
1:D:37:A:C2'	1:D:38:C:H5'	2.41	0.51
2:A:59:GLN:O	2:A:61:VAL:N	2.43	0.51
2:A:170:VAL:O	2:A:172:GLU:N	2.44	0.51
2:A:313:ARG:CB	2:A:313:ARG:HH11	2.24	0.51
2:A:350:ASN:HB2	2:A:355:LEU:HD11	1.93	0.51
1:D:16:A:H4'	1:D:16:A:OP1	2.11	0.51
2:A:353:VAL:CG1	2:A:354:CYS:N	2.74	0.51
2:B:74:PHE:O	2:B:77:GLU:HG2	2.11	0.51
2:B:111:PHE:C	2:B:111:PHE:HD2	2.19	0.51
2:B:313:ARG:HH11	2:B:313:ARG:HB3	1.75	0.51
2:A:20:VAL:HG23	2:A:182:ALA:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:LYS:NZ	2:B:175:LYS:HE2	2.26	0.51
2:B:174:GLU:C	2:B:176:PRO:HD2	2.36	0.51
1:C:8:U:H2'	1:C:8:U:O2	2.10	0.51
1:C:10:G:H2'	1:C:11:U:C6	2.45	0.51
1:D:15:G:O2'	1:D:16:A:OP1	2.28	0.51
2:A:8:VAL:CG2	2:A:30:TYR:CD2	2.93	0.51
2:A:217:GLN:O	2:A:217:GLN:HG2	2.11	0.51
2:B:180:LYS:O	2:B:181:ILE:C	2.53	0.51
2:A:76:ALA:HB3	2:A:77:GLU:OE1	2.10	0.50
2:A:156:TYR:CB	2:A:357:GLY:H	2.20	0.50
2:B:206:PHE:O	2:B:207:ARG:C	2.54	0.50
2:A:16:VAL:HG11	2:A:179:ARG:HG3	1.93	0.50
2:A:128:HIS:ND1	2:A:155:LEU:HD21	2.26	0.50
2:B:9:ILE:HD13	2:B:119:LEU:CD1	2.41	0.50
2:B:103:ASN:OD1	2:B:128:HIS:CE1	2.62	0.50
2:A:106:ILE:HA	2:A:110:ALA:HB3	1.92	0.50
2:B:149:LYS:HZ2	2:B:175:LYS:HE2	1.76	0.50
2:B:156:TYR:CD1	2:B:357:GLY:N	2.76	0.50
2:B:221:ILE:CG1	2:B:271:LEU:HD23	2.41	0.50
2:B:267:GLU:C	2:B:269:ASN:N	2.69	0.50
2:A:315:THR:O	2:A:316:ASP:C	2.55	0.50
2:B:255:THR:C	2:B:257:GLU:H	2.19	0.50
2:B:262:VAL:HG11	2:B:281:ARG:HB3	1.93	0.50
2:A:267:GLU:C	2:A:269:ASN:N	2.69	0.50
2:A:317:ILE:CD1	2:A:337:VAL:HG21	2.42	0.50
2:A:348:PHE:N	2:A:348:PHE:CD1	2.78	0.50
1:D:17:G:N2	1:D:55:U:O2	2.43	0.50
2:B:16:VAL:HG22	2:B:189:THR:O	2.11	0.50
2:B:170:VAL:C	2:B:172:GLU:N	2.66	0.50
2:B:222:ILE:HG22	2:B:223:THR:N	2.26	0.50
2:B:21:SER:OG	2:B:169:PRO:HG3	2.12	0.50
2:B:218:PRO:HA	2:B:233:GLN:HA	1.94	0.50
2:B:288:ILE:HD13	2:B:324:LEU:HD22	1.94	0.50
1:D:38:C:OP1	2:B:243:ARG:HB3	2.12	0.50
2:B:78:TYR:CE1	2:B:82:VAL:HG11	2.47	0.50
2:B:109:LYS:O	2:B:110:ALA:C	2.54	0.50
2:B:131:ARG:HB2	2:B:142:LEU:HD12	1.94	0.50
1:D:36:C:O2	2:B:311:ARG:NH2	2.45	0.50
2:A:61:VAL:HG12	2:A:65:LEU:HD12	1.94	0.50
2:B:159:SER:HB2	2:B:297:ARG:CG	2.41	0.50
2:A:341:THR:HG23	2:A:342:PRO:HD2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:G:H21	1:C:68:G:H1'	1.76	0.49
2:A:142:LEU:HB3	2:A:353:VAL:HA	1.94	0.49
2:A:206:PHE:O	2:A:207:ARG:C	2.54	0.49
2:B:27:GLN:C	2:B:29:GLY:H	2.20	0.49
2:B:252:LYS:HG2	2:B:253:GLU:HG3	1.93	0.49
1:C:36:C:H2'	1:C:37:A:O5'	2.11	0.49
1:D:36:C:H2'	1:D:37:A:O5'	2.12	0.49
2:A:141:LEU:HB2	2:A:163:ILE:HD11	1.93	0.49
1:D:34:U:OP1	2:B:312:TYR:OH	2.31	0.49
2:B:23:TRP:CZ3	2:B:24:LEU:HD23	2.48	0.49
1:D:8:U:H2'	1:D:8:U:O2	2.11	0.49
2:A:38:LYS:C	2:A:39:ASN:ND2	2.71	0.49
1:D:14:A:N6	1:D:21:A:C2	2.80	0.49
2:A:39:ASN:OD1	2:A:200:PHE:CE1	2.66	0.49
2:A:221:ILE:O	2:A:229:ILE:HG22	2.13	0.49
2:B:141:LEU:HB2	2:B:163:ILE:CD1	2.42	0.49
2:B:232:HIS:NE2	2:B:235:LEU:HD13	2.28	0.49
2:B:202:GLY:C	2:B:204:ARG:H	2.21	0.49
2:A:232:HIS:O	2:A:232:HIS:CG	2.66	0.49
2:B:73:ASN:ND2	2:B:75:ALA:CB	2.72	0.49
2:B:101:LEU:HD23	2:B:104:LYS:HD3	1.95	0.49
2:B:223:THR:CG2	2:B:224:VAL:N	2.74	0.49
2:B:315:THR:O	2:B:316:ASP:C	2.56	0.49
1:C:29:G:H2'	1:C:30:C:H6	1.78	0.49
2:A:122:ASP:O	2:A:123:TYR:CG	2.66	0.49
2:B:52:ALA:O	2:B:55:LEU:HB3	2.12	0.49
1:C:35:U:H2'	1:C:36:C:C6	2.47	0.49
2:A:289:ALA:HB3	2:A:329:ILE:HG13	1.95	0.49
2:B:130:VAL:HG22	2:B:131:ARG:H	1.78	0.49
1:D:15:G:O2'	1:D:16:A:P	2.70	0.48
2:B:232:HIS:O	2:B:234:GLY:O	2.29	0.48
1:D:24:A:H2'	1:D:25:C:H6	1.70	0.48
2:A:202:GLY:C	2:A:204:ARG:H	2.21	0.48
2:B:36:PHE:CD1	2:B:55:LEU:CD1	2.96	0.48
1:C:16:A:OP1	1:C:16:A:H4'	2.13	0.48
2:A:138:LYS:HG2	2:A:160:HIS:ND1	2.29	0.48
1:C:11:U:C2	1:C:12:C:C5	3.01	0.48
1:D:66:A:H3'	1:D:66:A:N3	2.29	0.48
2:A:310:THR:O	2:A:311:ARG:HG2	2.12	0.48
2:B:254:GLY:C	2:B:256:GLU:H	2.20	0.48
2:B:346:ALA:O	2:B:348:PHE:CE1	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:129:TYR:OH	2:B:146:ASP:HB2	2.13	0.48
2:B:156:TYR:CB	2:B:357:GLY:H	2.22	0.48
2:B:170:VAL:O	2:B:172:GLU:N	2.47	0.48
2:B:298:GLU:HG3	2:B:299:PRO:CD	2.39	0.48
2:B:26:GLN:NE2	2:B:67:ILE:HD11	2.29	0.48
2:B:122:ASP:OD1	2:B:122:ASP:N	2.47	0.48
2:A:35:LEU:HD11	2:A:72:VAL:CG2	2.32	0.48
2:B:7:LYS:HE2	2:B:33:GLU:CD	2.39	0.48
2:B:333:PHE:CD1	2:B:337:VAL:HG21	2.48	0.48
1:C:37:A:C2'	1:C:38:C:H5'	2.43	0.48
1:C:14:A:N6	1:C:21:A:C2	2.82	0.48
2:A:27:GLN:C	2:A:29:GLY:H	2.21	0.48
2:A:109:LYS:O	2:A:110:ALA:C	2.56	0.48
2:A:324:LEU:O	2:A:325:ASP:HB2	2.12	0.48
1:D:67:G:N3	1:D:67:G:H2'	2.29	0.48
2:A:100:ILE:CD1	2:A:154:PHE:HA	2.44	0.48
2:A:198:ILE:H	2:A:198:ILE:CD1	2.20	0.48
2:A:235:LEU:O	2:A:235:LEU:HD12	2.14	0.48
2:B:298:GLU:OE2	2:B:299:PRO:HD2	2.14	0.48
1:D:50:G:H2'	1:D:51:G:C8	2.49	0.47
2:B:14:GLY:O	2:B:189:THR:HG22	2.13	0.47
2:B:21:SER:OG	2:B:169:PRO:CG	2.62	0.47
2:A:217:GLN:O	2:A:218:PRO:O	2.31	0.47
1:C:2:U:H4'	1:C:3:C:C5	2.50	0.47
1:C:38:C:OP1	2:A:243:ARG:HB3	2.14	0.47
1:D:34:U:H5	2:B:154:PHE:CD1	2.31	0.47
2:A:111:PHE:CE1	2:A:124:ILE:CD1	2.97	0.47
2:A:130:VAL:CG2	2:A:131:ARG:N	2.75	0.47
2:A:292:LEU:HD13	2:A:294:TRP:HZ2	1.79	0.47
1:C:67:G:N3	1:C:67:G:H2'	2.29	0.47
2:A:139:SER:CB	2:A:164:ALA:HB2	2.45	0.47
2:A:139:SER:HB2	2:A:164:ALA:HB2	1.97	0.47
2:B:19:SER:CB	2:B:187:LEU:HD13	2.31	0.47
2:B:72:VAL:HG21	2:B:114:PHE:CE2	2.49	0.47
2:B:113:GLU:C	2:B:115:ALA:H	2.23	0.47
1:C:11:U:H2'	1:C:12:C:H6	1.77	0.47
1:C:22:G:O6	1:C:46:A:C2	2.67	0.47
1:D:29:G:H2'	1:D:30:C:H6	1.79	0.47
1:D:55:U:C6	1:D:57:G:OP2	2.68	0.47
2:A:254:GLY:C	2:A:256:GLU:H	2.22	0.47
2:A:311:ARG:HG3	2:A:311:ARG:HH11	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:GLN:O	2:B:218:PRO:O	2.31	0.47
2:B:333:PHE:HB3	2:B:335:GLU:O	2.14	0.47
2:B:100:ILE:HD11	2:B:156:TYR:CE2	2.49	0.47
2:B:223:THR:CG2	2:B:224:VAL:H	2.22	0.47
2:B:277:HIS:O	2:B:278:GLU:HB2	2.15	0.47
1:C:15:G:O2'	1:C:16:A:P	2.72	0.47
1:C:66:A:H3'	1:C:66:A:N3	2.29	0.47
1:D:17:G:H2'	1:D:57:G:N2	2.29	0.47
2:A:10:VAL:HA	2:A:125:ALA:O	2.15	0.47
2:A:24:LEU:O	2:A:28:GLN:HB2	2.14	0.47
2:B:45:GLY:C	2:B:47:GLU:N	2.72	0.47
2:B:196:THR:CG2	2:B:197:GLY:H	2.09	0.47
2:B:232:HIS:NE2	2:B:271:LEU:HB2	2.29	0.47
2:B:308:VAL:HG12	2:B:319:CYS:SG	2.54	0.47
2:A:111:PHE:CE2	2:A:124:ILE:HD11	2.49	0.47
2:B:122:ASP:O	2:B:123:TYR:CD2	2.68	0.47
2:B:130:VAL:O	2:B:171:GLY:HA3	2.15	0.47
2:B:175:LYS:CE	2:B:179:ARG:HH11	2.28	0.47
2:A:261:VAL:HG12	2:A:262:VAL:N	2.30	0.47
1:D:2:U:H4'	1:D:3:C:C5	2.50	0.47
2:A:198:ILE:HG21	2:A:201:ILE:HD12	1.97	0.47
2:A:224:VAL:HG12	2:A:224:VAL:O	2.15	0.47
2:B:130:VAL:CG2	2:B:131:ARG:N	2.77	0.47
2:B:193:LYS:O	2:B:194:ASP:C	2.58	0.47
1:C:29:G:H2'	1:C:30:C:C6	2.49	0.46
1:D:2:U:H4'	1:D:3:C:C4	2.50	0.46
2:B:27:GLN:HA	2:B:27:GLN:OE1	2.13	0.46
2:B:59:GLN:NE2	2:B:69:LEU:HB3	2.31	0.46
2:B:224:VAL:HG12	2:B:224:VAL:O	2.14	0.46
2:B:251:THR:O	2:B:253:GLU:N	2.48	0.46
2:A:260:TYR:CZ	2:A:277:HIS:HB2	2.50	0.46
2:B:20:VAL:HG21	2:B:178:VAL:O	2.16	0.46
1:C:2:U:H4'	1:C:3:C:C4	2.50	0.46
2:A:55:LEU:O	2:A:58:ALA:HB3	2.15	0.46
2:A:61:VAL:HG21	2:A:189:THR:HG23	1.97	0.46
2:B:262:VAL:HG11	2:B:281:ARG:HD3	1.98	0.46
1:D:9:C:N4	1:D:23:G:N7	2.61	0.46
2:A:130:VAL:O	2:A:171:GLY:HA3	2.16	0.46
2:B:111:PHE:CG	2:B:124:ILE:HD11	2.50	0.46
2:B:313:ARG:HB3	2:B:313:ARG:NH1	2.29	0.46
1:D:7:U:O2'	1:D:8:U:P	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:102:CYS:O	2:A:107:LYS:HE3	2.16	0.46
2:A:221:ILE:CG1	2:A:271:LEU:HD23	2.44	0.46
2:A:237:TYR:HB2	2:A:238:HIS:HD2	1.81	0.46
2:A:292:LEU:HD13	2:A:294:TRP:CZ2	2.50	0.46
2:B:10:VAL:HG12	2:B:125:ALA:CB	2.35	0.46
2:B:49:CYS:HA	2:B:52:ALA:HB3	1.98	0.46
2:B:274:ALA:O	2:B:275:GLN:HB2	2.16	0.46
2:B:26:GLN:HE22	2:B:65:LEU:HB3	1.80	0.46
2:B:198:ILE:HG21	2:B:201:ILE:HD12	1.98	0.46
2:A:304:MET:CG	2:A:305:ARG:N	2.79	0.46
2:B:131:ARG:HB2	2:B:131:ARG:HE	1.47	0.46
2:A:90:TYR:HE1	2:A:206:PHE:HZ	1.64	0.46
2:A:124:ILE:O	2:A:167:LEU:N	2.47	0.46
2:A:251:THR:O	2:A:253:GLU:N	2.48	0.46
2:B:197:GLY:O	2:B:198:ILE:C	2.57	0.46
2:B:265:ASP:CB	2:B:270:ILE:HB	2.46	0.46
1:D:22:G:O6	1:D:46:A:C2	2.68	0.46
2:A:113:GLU:C	2:A:115:ALA:H	2.24	0.46
2:A:193:LYS:O	2:A:194:ASP:C	2.59	0.46
2:A:194:ASP:O	2:A:195:SER:HB3	2.16	0.46
2:B:8:VAL:HG13	2:B:123:TYR:HB3	1.98	0.46
2:B:9:ILE:HD13	2:B:119:LEU:HD12	1.98	0.46
2:B:76:ALA:HB3	2:B:77:GLU:OE1	2.16	0.46
2:B:154:PHE:C	2:B:155:LEU:HD23	2.41	0.46
1:D:10:G:H2'	1:D:11:U:H6	1.80	0.46
1:D:11:U:C2	1:D:12:C:C5	3.03	0.46
2:A:180:LYS:HA	2:A:180:LYS:HD3	1.76	0.46
2:A:304:MET:HG3	2:A:305:ARG:N	2.31	0.46
2:B:51:ALA:HA	2:B:54:ASP:HB2	1.98	0.46
2:B:232:HIS:CE1	2:B:235:LEU:HA	2.42	0.46
2:B:324:LEU:O	2:B:325:ASP:HB2	2.15	0.46
1:C:10:G:H2'	1:C:11:U:H6	1.81	0.45
1:D:34:U:C5	2:B:154:PHE:CD1	3.04	0.45
2:A:290:GLN:O	2:A:292:LEU:CD2	2.64	0.45
2:B:353:VAL:CG1	2:B:354:CYS:N	2.80	0.45
1:D:67:G:N2	1:D:68:G:H1'	2.31	0.45
2:A:111:PHE:CE1	2:A:124:ILE:CG1	2.99	0.45
2:B:10:VAL:HA	2:B:125:ALA:O	2.15	0.45
2:B:232:HIS:CE1	2:B:235:LEU:HB2	2.51	0.45
2:A:73:ASN:C	2:A:73:ASN:ND2	2.74	0.45
2:A:260:TYR:CE2	2:A:277:HIS:N	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:287:LEU:HD22	2:A:340:VAL:HG11	1.98	0.45
2:B:260:TYR:CZ	2:B:277:HIS:HB2	2.51	0.45
1:C:34:U:H2'	1:C:35:U:H5''	1.99	0.45
1:D:35:U:H2'	1:D:36:C:C6	2.51	0.45
2:A:19:SER:O	2:A:20:VAL:C	2.58	0.45
2:A:51:ALA:HA	2:A:54:ASP:HB2	1.97	0.45
2:A:85:LEU:N	2:A:85:LEU:HD23	2.31	0.45
2:A:265:ASP:CB	2:A:270:ILE:HB	2.44	0.45
2:B:128:HIS:ND1	2:B:155:LEU:HD21	2.32	0.45
2:B:192:LYS:O	2:B:193:LYS:C	2.59	0.45
2:B:319:CYS:HB2	2:B:331:VAL:CG1	2.46	0.45
1:D:4:C:O2	1:D:69:G:N2	2.49	0.45
2:A:114:PHE:O	2:A:114:PHE:CD2	2.69	0.45
2:A:115:ALA:O	2:A:120:GLY:N	2.49	0.45
2:A:350:ASN:OD1	2:A:350:ASN:O	2.34	0.45
2:B:111:PHE:O	2:B:112:LEU:C	2.60	0.45
1:C:9:C:N4	1:C:23:G:N7	2.63	0.45
1:C:16:A:N3	1:C:16:A:H2'	2.32	0.45
1:C:50:G:H2'	1:C:51:G:C8	2.51	0.45
2:B:16:VAL:HG11	2:B:179:ARG:HG3	1.98	0.45
2:B:19:SER:O	2:B:20:VAL:C	2.57	0.45
2:A:45:GLY:C	2:A:47:GLU:N	2.73	0.45
2:A:132:ARG:HD2	2:A:163:ILE:HG23	1.98	0.45
2:A:206:PHE:CE2	2:A:210:LEU:HB2	2.51	0.45
2:B:115:ALA:O	2:B:120:GLY:N	2.50	0.45
2:B:205:LYS:HD2	2:B:207:ARG:NE	2.32	0.45
2:B:353:VAL:HG12	2:B:354:CYS:N	2.32	0.45
2:B:181:ILE:O	2:B:185:LEU:HG	2.17	0.45
2:A:192:LYS:O	2:A:193:LYS:C	2.59	0.45
2:B:190:ALA:O	2:B:191:LYS:CB	2.65	0.45
1:D:29:G:H2'	1:D:30:C:C6	2.51	0.45
2:A:288:ILE:HD11	2:A:330:GLU:CB	2.47	0.45
2:A:306:CYS:HB2	2:A:349:TYR:O	2.16	0.45
2:B:90:TYR:HE1	2:B:206:PHE:HZ	1.65	0.45
1:C:15:G:H4'	1:C:16:A:OP2	2.17	0.44
2:A:74:PHE:O	2:A:75:ALA:C	2.61	0.44
2:A:325:ASP:CG	2:A:326:ASP:H	2.25	0.44
2:B:341:THR:HG23	2:B:342:PRO:HD2	1.99	0.44
1:C:17:G:H2'	1:C:57:G:N2	2.32	0.44
1:C:32:C:C4	1:C:33:U:C4	3.05	0.44
2:A:20:VAL:HG21	2:A:178:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:99:ASP:OD1	2:A:199:CYS:N	2.41	0.44
2:A:156:TYR:CD1	2:A:357:GLY:CA	3.01	0.44
2:A:189:THR:O	2:A:190:ALA:C	2.59	0.44
2:A:197:GLY:O	2:A:198:ILE:C	2.59	0.44
2:A:222:ILE:HG22	2:A:223:THR:N	2.32	0.44
2:A:363:ARG:O	2:A:364:LEU:HD23	2.17	0.44
2:B:83:PHE:C	2:B:86:PHE:HB3	2.42	0.44
2:B:131:ARG:NH2	2:B:142:LEU:HD13	2.14	0.44
2:B:175:LYS:HE3	2:B:179:ARG:HH11	1.83	0.44
1:C:67:G:N2	1:C:68:G:H1'	2.32	0.44
1:D:9:C:C6	1:D:11:U:O4	2.71	0.44
1:D:16:A:N3	1:D:16:A:H2'	2.31	0.44
2:A:200:PHE:N	2:A:200:PHE:CD2	2.85	0.44
2:B:27:GLN:C	2:B:29:GLY:N	2.75	0.44
2:A:190:ALA:O	2:A:191:LYS:CB	2.65	0.44
2:B:57:ASP:O	2:B:61:VAL:HG23	2.18	0.44
2:A:89:GLU:OE2	2:A:94:ARG:NH1	2.51	0.44
2:A:108:PHE:CG	2:A:158:LEU:HD21	2.52	0.44
2:A:199:CYS:O	2:A:200:PHE:CB	2.66	0.44
2:A:202:GLY:HA3	2:A:204:ARG:HH21	1.82	0.44
2:A:333:PHE:CE2	2:A:337:VAL:HB	2.53	0.44
2:B:289:ALA:O	2:B:328:ARG:HA	2.18	0.44
2:A:143:ARG:HB2	2:A:150:ASP:OD2	2.17	0.44
2:A:248:ILE:HD13	2:A:259:TRP:CE3	2.53	0.44
2:B:29:GLY:O	2:B:30:TYR:O	2.36	0.44
2:B:42:GLU:HB3	2:B:47:GLU:HG2	2.00	0.44
2:B:178:VAL:C	2:B:180:LYS:H	2.25	0.44
1:C:25:C:H2'	1:C:26:A:O4'	2.18	0.44
1:D:66:A:H2	1:D:67:G:N7	2.16	0.44
2:A:295:VAL:CG1	2:A:296:ASP:N	2.81	0.44
2:B:27:GLN:O	2:B:29:GLY:N	2.50	0.44
2:B:178:VAL:C	2:B:180:LYS:N	2.75	0.44
2:B:262:VAL:O	2:B:263:ASP:CG	2.61	0.44
2:B:287:LEU:C	2:B:287:LEU:CD1	2.89	0.44
2:B:287:LEU:HD23	2:B:340:VAL:HG11	1.99	0.44
1:C:36:C:C2'	1:C:37:A:O5'	2.65	0.44
1:C:67:G:H8	1:C:67:G:OP2	2.01	0.44
1:D:9:C:H4'	1:D:46:A:O4'	2.17	0.44
2:A:53:ALA:C	2:A:55:LEU:N	2.74	0.44
2:A:132:ARG:HD2	2:A:163:ILE:CG2	2.47	0.44
1:D:8:U:C2	1:D:15:G:O6	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:C:C2'	1:D:37:A:O5'	2.66	0.44
2:A:106:ILE:HG22	2:A:107:LYS:N	2.33	0.44
2:A:143:ARG:CB	2:A:150:ASP:OD2	2.66	0.44
2:A:160:HIS:O	2:A:161:GLU:C	2.61	0.44
2:B:89:GLU:HG2	2:B:94:ARG:HH22	1.74	0.44
2:B:292:LEU:HD11	2:B:329:ILE:HG23	1.99	0.44
3:C:134:AMP:O2'	2:A:126:THR:HA	2.18	0.43
2:A:27:GLN:O	2:A:29:GLY:N	2.51	0.43
2:A:350:ASN:CB	2:A:355:LEU:HD21	2.48	0.43
2:B:8:VAL:HG21	2:B:30:TYR:CD2	2.53	0.43
2:B:122:ASP:O	2:B:123:TYR:CG	2.71	0.43
2:B:303:THR:HG23	2:B:321:VAL:O	2.18	0.43
2:A:312:TYR:O	2:A:313:ARG:C	2.61	0.43
2:B:74:PHE:HZ	2:B:114:PHE:HB2	1.84	0.43
2:B:233:GLN:C	2:B:233:GLN:OE1	2.61	0.43
2:B:295:VAL:O	2:B:297:ARG:HG2	2.17	0.43
1:C:7:U:O4	1:C:49:A:N6	2.51	0.43
2:A:35:LEU:HD21	2:A:72:VAL:HB	2.01	0.43
2:B:53:ALA:C	2:B:55:LEU:N	2.74	0.43
2:B:160:HIS:O	2:B:161:GLU:C	2.60	0.43
2:B:292:LEU:HD21	2:B:329:ILE:HD13	1.99	0.43
2:B:312:TYR:CG	2:B:313:ARG:N	2.86	0.43
1:C:22:G:O6	1:C:46:A:N1	2.51	0.43
3:C:134:AMP:H4'	2:A:128:HIS:CD2	2.54	0.43
1:D:20:C:C5'	1:D:20(A):C:OP1	2.62	0.43
2:A:220:LYS:O	2:A:232:HIS:HB2	2.17	0.43
2:A:249:GLY:O	2:A:250:GLY:O	2.36	0.43
2:A:308:VAL:HG12	2:A:319:CYS:SG	2.58	0.43
2:A:313:ARG:HB3	2:A:313:ARG:NH1	2.33	0.43
2:B:39:ASN:HA	2:B:75:ALA:HB2	1.99	0.43
2:B:59:GLN:C	2:B:61:VAL:H	2.26	0.43
2:B:102:CYS:HG	2:B:107:LYS:NZ	2.14	0.43
1:C:8:U:C2	1:C:15:G:O6	2.72	0.43
2:A:220:LYS:C	2:A:232:HIS:HB2	2.43	0.43
2:A:292:LEU:HD21	2:A:329:ILE:HD11	2.01	0.43
2:A:333:PHE:HB3	2:A:335:GLU:O	2.19	0.43
1:D:35:U:C2	2:B:97:ASN:ND2	2.87	0.43
2:A:114:PHE:O	2:A:114:PHE:CG	2.71	0.43
2:A:305:ARG:NH1	2:A:320:THR:OG1	2.52	0.43
2:B:42:GLU:HG2	2:B:48:TYR:HA	1.99	0.43
2:B:74:PHE:O	2:B:75:ALA:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:GLY:O	2:B:187:LEU:C	2.60	0.43
2:B:245:GLY:C	2:B:246:LEU:HD23	2.44	0.43
2:A:297:ARG:HD3	2:A:297:ARG:HA	1.84	0.43
2:B:156:TYR:HD1	2:B:357:GLY:N	2.15	0.43
2:B:217:GLN:HA	2:B:218:PRO:HD2	1.91	0.43
2:B:312:TYR:O	2:B:313:ARG:C	2.61	0.43
1:D:32:C:C4	1:D:33:U:C4	3.06	0.43
2:A:30:TYR:CE2	2:A:167:LEU:HD11	2.54	0.43
2:A:98:PRO:O	2:A:99:ASP:C	2.62	0.43
2:A:107:LYS:HE2	2:A:200:PHE:CZ	2.51	0.43
2:A:289:ALA:O	2:A:328:ARG:HA	2.18	0.43
2:A:363:ARG:HG3	2:A:365:PRO:HD3	2.00	0.43
2:B:83:PHE:CE1	2:B:87:LEU:HD11	2.47	0.43
2:B:114:PHE:O	2:B:114:PHE:CG	2.72	0.43
2:B:294:TRP:O	2:B:297:ARG:N	2.49	0.43
3:D:134:AMP:H4'	2:B:128:HIS:HD2	1.83	0.43
2:B:82:VAL:HG12	2:B:83:PHE:N	2.32	0.43
2:B:101:LEU:C	2:B:103:ASN:N	2.74	0.43
2:B:304:MET:HB3	2:B:321:VAL:HB	2.01	0.43
2:A:154:PHE:HE1	2:A:312:TYR:CD1	2.37	0.43
2:A:199:CYS:SG	2:A:200:PHE:CD2	3.08	0.43
2:A:254:GLY:O	2:A:256:GLU:N	2.52	0.43
2:A:307:THR:OG1	2:A:308:VAL:N	2.50	0.43
3:D:134:AMP:O2'	2:B:126:THR:HA	2.19	0.42
2:A:149:LYS:NZ	2:A:175:LYS:HE2	2.34	0.42
2:A:202:GLY:HA3	2:A:204:ARG:HE	1.83	0.42
2:B:24:LEU:HD11	2:B:173:LEU:HD11	2.00	0.42
2:B:232:HIS:CD2	2:B:270:ILE:C	2.97	0.42
2:B:268:ASN:O	2:B:269:ASN:C	2.61	0.42
2:B:290:GLN:O	2:B:292:LEU:HG	2.19	0.42
1:C:4:C:O2	1:C:69:G:N2	2.52	0.42
1:C:9:C:C6	1:C:11:U:O4	2.71	0.42
1:C:38:C:O2	1:C:38:C:O4'	2.37	0.42
2:A:237:TYR:HB2	2:A:238:HIS:CD2	2.54	0.42
2:A:268:ASN:O	2:A:269:ASN:C	2.62	0.42
2:B:59:GLN:C	2:B:61:VAL:N	2.76	0.42
2:B:74:PHE:HA	2:B:77:GLU:OE1	2.19	0.42
2:B:87:LEU:CD1	2:B:213:TYR:HB3	2.48	0.42
2:B:333:PHE:CE1	2:B:337:VAL:HG21	2.54	0.42
1:C:56:C:H6	1:C:56:C:O5'	2.02	0.42
2:A:29:GLY:O	2:A:30:TYR:O	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:178:VAL:C	2:A:180:LYS:N	2.77	0.42
2:B:149:LYS:HD2	2:B:175:LYS:HG2	2.02	0.42
2:B:286:GLY:CA	2:B:364:LEU:HD12	2.48	0.42
1:C:23:G:O2'	1:C:24:A:H5'	2.18	0.42
1:C:38:C:O2	1:C:38:C:O5'	2.37	0.42
1:D:34:U:H3'	1:D:34:U:H6	1.84	0.42
2:A:21:SER:HB2	2:A:170:VAL:HG13	2.01	0.42
2:B:35:LEU:C	2:B:35:LEU:CD2	2.91	0.42
2:B:151:GLN:O	2:B:152:SER:C	2.60	0.42
2:B:219:GLY:CA	2:B:232:HIS:HB3	2.50	0.42
2:B:265:ASP:O	2:B:266:VAL:C	2.62	0.42
2:B:364:LEU:HA	2:B:364:LEU:HD23	1.80	0.42
1:D:31:C:H2'	1:D:32:C:H6	1.85	0.42
2:A:25:LEU:HD23	2:A:28:GLN:HE22	1.82	0.42
2:A:27:GLN:C	2:A:29:GLY:N	2.76	0.42
2:A:83:PHE:C	2:A:86:PHE:HB3	2.45	0.42
2:A:319:CYS:HB2	2:A:331:VAL:HG12	2.01	0.42
2:B:131:ARG:HB2	2:B:142:LEU:CD1	2.49	0.42
1:C:7:U:O2'	1:C:8:U:P	2.77	0.42
1:C:34:U:H3'	1:C:34:U:H6	1.85	0.42
2:A:9:ILE:HD13	2:A:119:LEU:CB	2.50	0.42
2:A:26:GLN:HE22	2:A:65:LEU:HB3	1.84	0.42
2:A:111:PHE:O	2:A:112:LEU:C	2.61	0.42
2:A:186:GLY:O	2:A:187:LEU:C	2.62	0.42
2:B:307:THR:HG23	2:B:349:TYR:O	2.19	0.42
1:D:49:A:H2'	1:D:50:G:C8	2.55	0.42
2:B:111:PHE:CE1	2:B:124:ILE:HD11	2.55	0.42
2:B:254:GLY:O	2:B:256:GLU:N	2.51	0.42
1:D:9:C:O2'	1:D:45:A:O2'	2.18	0.42
2:A:57:ASP:O	2:A:61:VAL:HG23	2.20	0.42
2:A:73:ASN:ND2	2:A:75:ALA:H	2.17	0.42
2:A:221:ILE:HB	2:A:230:GLY:O	2.18	0.42
2:A:294:TRP:O	2:A:297:ARG:N	2.50	0.42
2:B:199:CYS:O	2:B:200:PHE:CB	2.67	0.42
1:C:20:C:H1'	1:C:21:A:O4'	2.18	0.42
1:C:55:U:H2'	1:C:57:G:N7	2.35	0.42
1:D:24:A:C5	1:D:25:C:C4	3.08	0.42
2:A:143:ARG:HB3	2:A:152:SER:OG	2.20	0.42
2:B:8:VAL:HG21	2:B:30:TYR:CB	2.48	0.42
2:B:8:VAL:HG13	2:B:123:TYR:CB	2.50	0.42
1:C:9:C:H4'	1:C:46:A:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:173:LEU:CD1	2:A:178:VAL:HG22	2.49	0.42
2:A:265:ASP:O	2:A:266:VAL:C	2.62	0.42
2:B:77:GLU:H	2:B:77:GLU:CD	2.28	0.42
2:B:210:LEU:C	2:B:212:ARG:H	2.28	0.42
2:B:220:LYS:O	2:B:232:HIS:HB2	2.20	0.42
2:A:109:LYS:HB3	2:A:110:ALA:H	1.74	0.41
2:A:139:SER:OG	2:A:163:ILE:HG22	2.20	0.41
2:B:107:LYS:NZ	2:B:199:CYS:SG	2.92	0.41
2:B:232:HIS:HE1	2:B:235:LEU:CA	2.27	0.41
3:C:134:AMP:H4'	2:A:128:HIS:HD2	1.85	0.41
2:A:59:GLN:HA	2:A:69:LEU:HD22	2.00	0.41
2:A:312:TYR:CG	2:A:313:ARG:N	2.88	0.41
2:B:189:THR:O	2:B:190:ALA:C	2.60	0.41
2:B:189:THR:O	2:B:192:LYS:HB2	2.20	0.41
1:D:15:G:O2'	1:D:59:A:N1	2.48	0.41
2:A:160:HIS:CD2	2:A:161:GLU:HG2	2.54	0.41
2:A:229:ILE:HG23	2:A:230:GLY:N	2.35	0.41
2:A:255:THR:C	2:A:257:GLU:N	2.79	0.41
1:C:66:A:H2	1:C:67:G:N7	2.18	0.41
2:A:42:GLU:HB3	2:A:47:GLU:HG2	2.03	0.41
2:A:106:ILE:C	2:A:108:PHE:N	2.78	0.41
2:A:200:PHE:N	2:A:200:PHE:HD2	2.17	0.41
2:A:287:LEU:CD2	2:A:340:VAL:HG11	2.50	0.41
2:A:287:LEU:HD13	2:A:360:ILE:HG12	2.02	0.41
2:B:160:HIS:CD2	2:B:161:GLU:HG2	2.55	0.41
1:D:38:C:O2	1:D:38:C:O5'	2.38	0.41
2:A:268:ASN:HB2	2:A:270:ILE:HG13	2.02	0.41
2:B:106:ILE:C	2:B:108:PHE:N	2.78	0.41
2:B:193:LYS:C	2:B:195:SER:N	2.79	0.41
2:A:210:LEU:C	2:A:212:ARG:H	2.28	0.41
2:B:98:PRO:HB2	2:B:198:ILE:HG23	2.01	0.41
2:B:98:PRO:O	2:B:99:ASP:C	2.61	0.41
2:B:100:ILE:CG1	2:B:156:TYR:CE2	3.02	0.41
2:B:255:THR:C	2:B:257:GLU:N	2.79	0.41
2:B:331:VAL:HG21	2:B:348:PHE:CE2	2.56	0.41
2:A:48:TYR:CE2	2:A:52:ALA:HB2	2.56	0.41
2:A:73:ASN:ND2	2:A:75:ALA:HB3	2.32	0.41
2:A:282:LEU:HD12	2:A:282:LEU:HA	1.84	0.41
2:B:325:ASP:CG	2:B:326:ASP:H	2.29	0.41
1:D:67:G:H8	1:D:67:G:OP2	2.03	0.41
2:A:94:ARG:HH11	2:A:361:GLU:CD	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:GLN:HE21	2:B:26:GLN:HB2	1.71	0.41
2:B:311:ARG:HH12	2:B:341:THR:HB	1.84	0.41
1:C:55:U:C6	1:C:57:G:OP2	2.73	0.41
2:A:21:SER:OG	2:A:169:PRO:CG	2.68	0.41
2:A:55:LEU:O	2:A:58:ALA:N	2.54	0.41
2:A:59:GLN:C	2:A:61:VAL:H	2.29	0.41
2:A:128:HIS:CE1	2:A:155:LEU:HD21	2.56	0.41
2:A:221:ILE:HB	2:A:230:GLY:C	2.45	0.41
2:B:139:SER:CB	2:B:164:ALA:HB2	2.51	0.41
2:B:175:LYS:HE3	2:B:179:ARG:HD3	2.03	0.41
2:B:249:GLY:O	2:B:250:GLY:O	2.39	0.41
1:D:44:U:H2'	1:D:45:A:O4'	2.20	0.41
2:A:59:GLN:C	2:A:61:VAL:N	2.77	0.41
2:B:49:CYS:O	2:B:50:THR:C	2.64	0.41
1:C:20:C:C5'	1:C:20(A):C:OP1	2.63	0.40
1:C:24:A:C5	1:C:25:C:C4	3.09	0.40
1:D:22:G:O6	1:D:46:A:N1	2.54	0.40
2:A:185:LEU:HB2	2:A:187:LEU:HG	2.02	0.40
2:B:142:LEU:HB3	2:B:353:VAL:HA	2.03	0.40
2:B:210:LEU:CD2	2:B:236:MET:HG3	2.50	0.40
2:B:221:ILE:HB	2:B:230:GLY:O	2.21	0.40
1:C:49:A:N1	1:C:66:A:N6	2.69	0.40
1:D:15:G:H4'	1:D:16:A:OP2	2.21	0.40
2:A:193:LYS:C	2:A:195:SER:N	2.78	0.40
2:A:210:LEU:HD12	2:A:210:LEU:HA	1.88	0.40
2:A:305:ARG:HA	2:A:305:ARG:HD2	1.93	0.40
2:B:294:TRP:O	2:B:295:VAL:C	2.63	0.40
2:A:12:MET:HG3	2:A:62:CYS:SG	2.61	0.40
2:A:72:VAL:HG12	2:A:73:ASN:N	2.35	0.40
2:A:277:HIS:O	2:A:278:GLU:CG	2.63	0.40
2:A:294:TRP:O	2:A:295:VAL:C	2.63	0.40
2:B:10:VAL:CG1	2:B:125:ALA:HB3	2.38	0.40
2:B:36:PHE:CE1	2:B:55:LEU:HB2	2.56	0.40
2:B:113:GLU:C	2:B:115:ALA:N	2.79	0.40
2:B:258:PRO:HG2	2:B:260:TYR:CE1	2.56	0.40
2:A:225:ASP:O	2:A:227:ASP:OD1	2.40	0.40
2:A:259:TRP:HE3	2:A:273:VAL:CG2	2.34	0.40
2:A:292:LEU:HD11	2:A:329:ILE:CG1	2.50	0.40
2:A:294:TRP:O	2:A:297:ARG:HD3	2.22	0.40
2:B:146:ASP:OD2	2:B:175:LYS:N	2.55	0.40
3:D:134:AMP:O2'	2:B:126:THR:HB	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:126:THR:HB	2:A:128:HIS:CD2	2.57	0.40
2:A:178:VAL:C	2:A:180:LYS:H	2.30	0.40
2:B:153:TYR:HA	2:B:347:VAL:HG21	2.02	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	362/380 (95%)	246 (68%)	71 (20%)	45 (12%)	0	1
2	B	362/380 (95%)	243 (67%)	76 (21%)	43 (12%)	0	2
All	All	724/760 (95%)	489 (68%)	147 (20%)	88 (12%)	0	1

All (88) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	30	TYR
2	A	48	TYR
2	A	147	SER
2	A	218	PRO
2	A	247	GLY
2	A	252	LYS
2	A	266	VAL
2	A	278	GLU
2	A	291	GLN
2	B	17	ASP
2	B	30	TYR
2	B	48	TYR
2	B	194	ASP
2	B	218	PRO
2	B	247	GLY

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Mol	Chain	Res	Type
2	B	252	LYS
2	B	266	VAL
2	B	278	GLU
2	B	291	GLN
2	A	17	ASP
2	A	60	ALA
2	A	88	ALA
2	A	107	LYS
2	A	194	ASP
2	A	195	SER
2	A	226	GLY
2	A	229	ILE
2	A	233	GLN
2	A	250	GLY
2	A	255	THR
2	A	316	ASP
2	A	325	ASP
2	B	60	ALA
2	B	107	LYS
2	B	147	SER
2	B	195	SER
2	B	226	GLY
2	B	229	ILE
2	B	233	GLN
2	B	250	GLY
2	B	255	THR
2	B	316	ASP
2	B	325	ASP
2	A	18	SER
2	A	28	GLN
2	A	112	LEU
2	A	114	PHE
2	A	191	LYS
2	A	193	LYS
2	A	197	GLY
2	A	207	ARG
2	A	274	ALA
2	A	318	PRO
2	A	365	PRO
2	B	18	SER
2	B	28	GLN
2	B	88	ALA

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Mol	Chain	Res	Type
2	B	114	PHE
2	B	191	LYS
2	B	193	LYS
2	B	197	GLY
2	B	207	ARG
2	B	274	ALA
2	B	318	PRO
2	B	365	PRO
2	A	111	PHE
2	A	203	GLU
2	A	206	PHE
2	A	215	PRO
2	A	235	LEU
2	A	313	ARG
2	A	314	GLN
2	B	112	LEU
2	B	203	GLU
2	B	206	PHE
2	B	215	PRO
2	B	235	LEU
2	B	313	ARG
2	B	314	GLN
2	A	109	LYS
2	A	173	LEU
2	B	109	LYS
2	B	173	LEU
2	B	232	HIS
2	A	19	SER
2	B	111	PHE
2	A	169	PRO
2	A	171	GLY

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	301/315 (96%)	276 (92%)	25 (8%)	10	35
2	B	301/315 (96%)	267 (89%)	34 (11%)	5	21
All	All	602/630 (96%)	543 (90%)	59 (10%)	7	27

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	42	GLU
2	A	54	ASP
2	A	77	GLU
2	A	80	ASP
2	A	85	LEU
2	A	90	TYR
2	A	146	ASP
2	A	150	ASP
2	A	188	VAL
2	A	204	ARG
2	A	206	PHE
2	A	233	GLN
2	A	239	THR
2	A	255	THR
2	A	261	VAL
2	A	263	ASP
2	A	288	ILE
2	A	307	THR
2	A	313	ARG
2	A	315	THR
2	A	326	ASP
2	A	329	ILE
2	A	334	ASP
2	A	348	PHE
2	A	365	PRO
2	B	8	VAL
2	B	9	ILE
2	B	20	VAL
2	B	35	LEU
2	B	36	PHE
2	B	37	MET
2	B	39	ASN

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Mol	Chain	Res	Type
2	B	42	GLU
2	B	77	GLU
2	B	80	ASP
2	B	85	LEU
2	B	90	TYR
2	B	96	PRO
2	B	101	LEU
2	B	111	PHE
2	B	140	ARG
2	B	148	ASN
2	B	150	ASP
2	B	160	HIS
2	B	179	ARG
2	B	188	VAL
2	B	204	ARG
2	B	206	PHE
2	B	233	GLN
2	B	239	THR
2	B	307	THR
2	B	313	ARG
2	B	315	THR
2	B	318	PRO
2	B	332	ILE
2	B	334	ASP
2	B	348	PHE
2	B	355	LEU
2	B	363	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	26	GLN
2	A	28	GLN
2	A	39	ASN
2	A	59	GLN
2	A	73	ASN
2	A	148	ASN
2	A	160	HIS
2	A	233	GLN
2	A	238	HIS
2	A	275	GLN
2	A	344	GLN

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Mol	Chain	Res	Type
2	A	350	ASN
2	B	26	GLN
2	B	28	GLN
2	B	39	ASN
2	B	59	GLN
2	B	73	ASN
2	B	97	ASN
2	B	128	HIS
2	B	148	ASN
2	B	160	HIS
2	B	162	GLN
2	B	269	ASN
2	B	275	GLN
2	B	279	HIS
2	B	350	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	73/76 (96%)	23 (31%)	6 (8%)
1	D	73/76 (96%)	23 (31%)	6 (8%)
All	All	146/152 (96%)	46 (31%)	12 (8%)

All (46) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	3	C
1	C	4	C
1	C	6	C
1	C	8	U
1	C	9	C
1	C	10	G
1	C	16	A
1	C	17	G
1	C	19	C
1	C	20(A)	C
1	C	34	U
1	C	35	U
1	C	37	A
1	C	47	C
1	C	49	A

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Mol	Chain	Res	Type
1	C	58	A
1	C	61	C
1	C	65	U
1	C	66	A
1	C	67	G
1	C	71	A
1	C	73	G
1	C	74	C
1	D	3	C
1	D	4	C
1	D	6	C
1	D	8	U
1	D	9	C
1	D	10	G
1	D	16	A
1	D	17	G
1	D	19	C
1	D	20(A)	C
1	D	34	U
1	D	35	U
1	D	37	A
1	D	47	C
1	D	49	A
1	D	58	A
1	D	61	C
1	D	65	U
1	D	66	A
1	D	67	G
1	D	71	A
1	D	73	G
1	D	74	C

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	7	U
1	C	9	C
1	C	15	G
1	C	18	G
1	C	20	C
1	C	34	U
1	D	7	U

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Mol	Chain	Res	Type
1	D	9	C
1	D	15	G
1	D	18	G
1	D	20	C
1	D	34	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	AMP	C	134	1	21,24,25	0.73	0	30,35,38	0.48	0
3	AMP	D	134	1	21,24,25	0.77	0	30,35,38	0.49	0
4	SO4	B	5002	-	4,4,4	1.31	0	6,6,6	0.50	0
4	SO4	A	5001	-	4,4,4	1.32	0	6,6,6	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	C	134	1	-	2/7/25/26	0/3/3/3
3	AMP	D	134	1	-	2/7/25/26	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

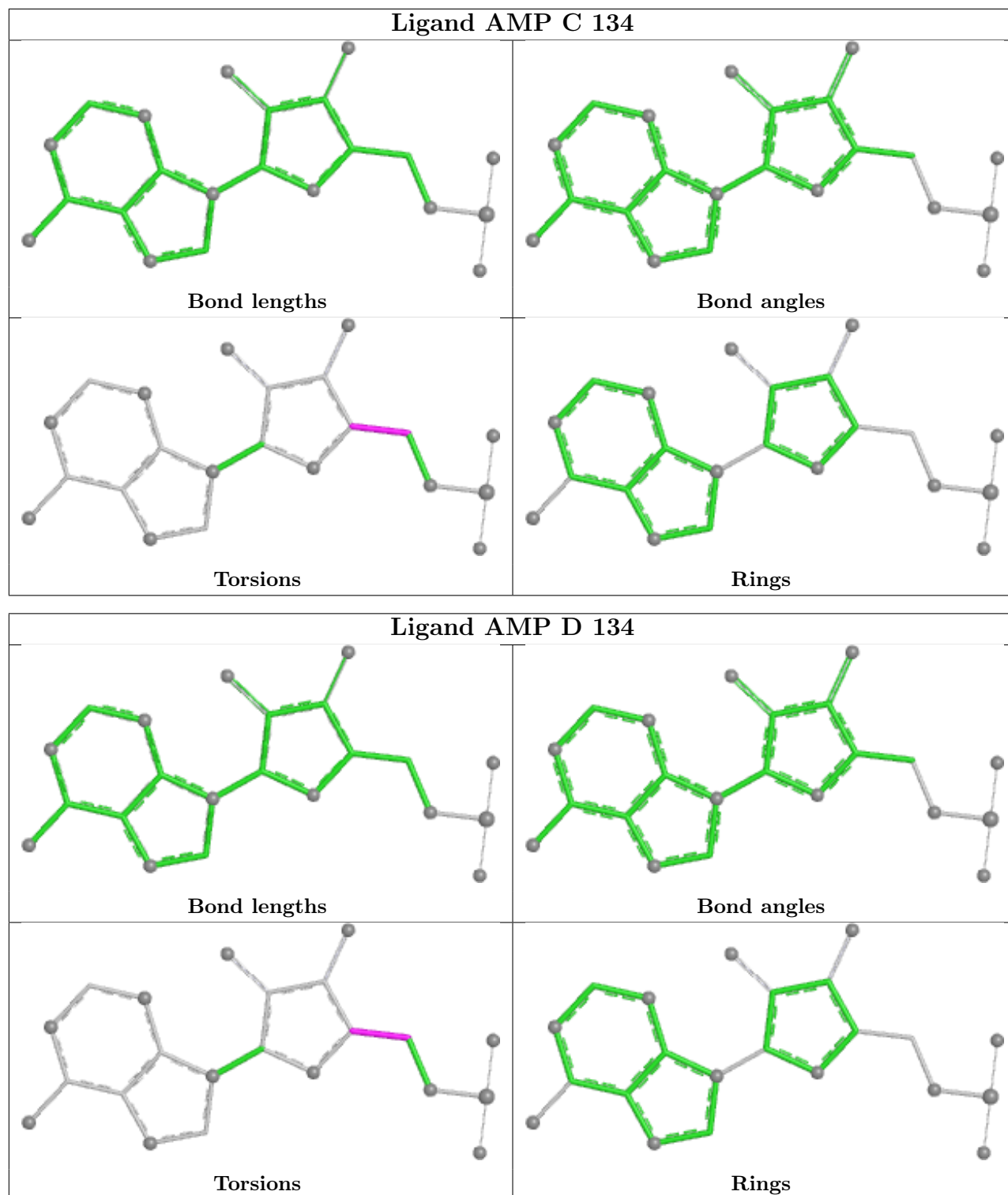
Mol	Chain	Res	Type	Atoms
3	C	134	AMP	O4'-C4'-C5'-O5'
3	D	134	AMP	O4'-C4'-C5'-O5'
3	C	134	AMP	C3'-C4'-C5'-O5'
3	D	134	AMP	C3'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	134	AMP	3	0
3	D	134	AMP	4	0
4	B	5002	SO4	2	0
4	A	5001	SO4	1	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 than 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.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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	74/76 (97%)	-0.98	1 (1%) 73 59	45, 86, 197, 200	0
1	D	74/76 (97%)	-1.00	1 (1%) 73 59	52, 83, 198, 200	0
2	A	364/380 (95%)	-0.67	5 (1%) 73 59	32, 83, 142, 172	0
2	B	364/380 (95%)	-0.73	1 (0%) 90 84	33, 83, 140, 173	0
All	All	876/912 (96%)	-0.75	8 (0%) 81 68	32, 83, 156, 200	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	73	G	4.2
2	A	194	ASP	3.0
2	A	250	GLY	3.0
2	B	312	TYR	2.8
2	A	195	SER	2.7
1	D	73	G	2.5
2	A	249	GLY	2.2
2	A	361	GLU	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](#)

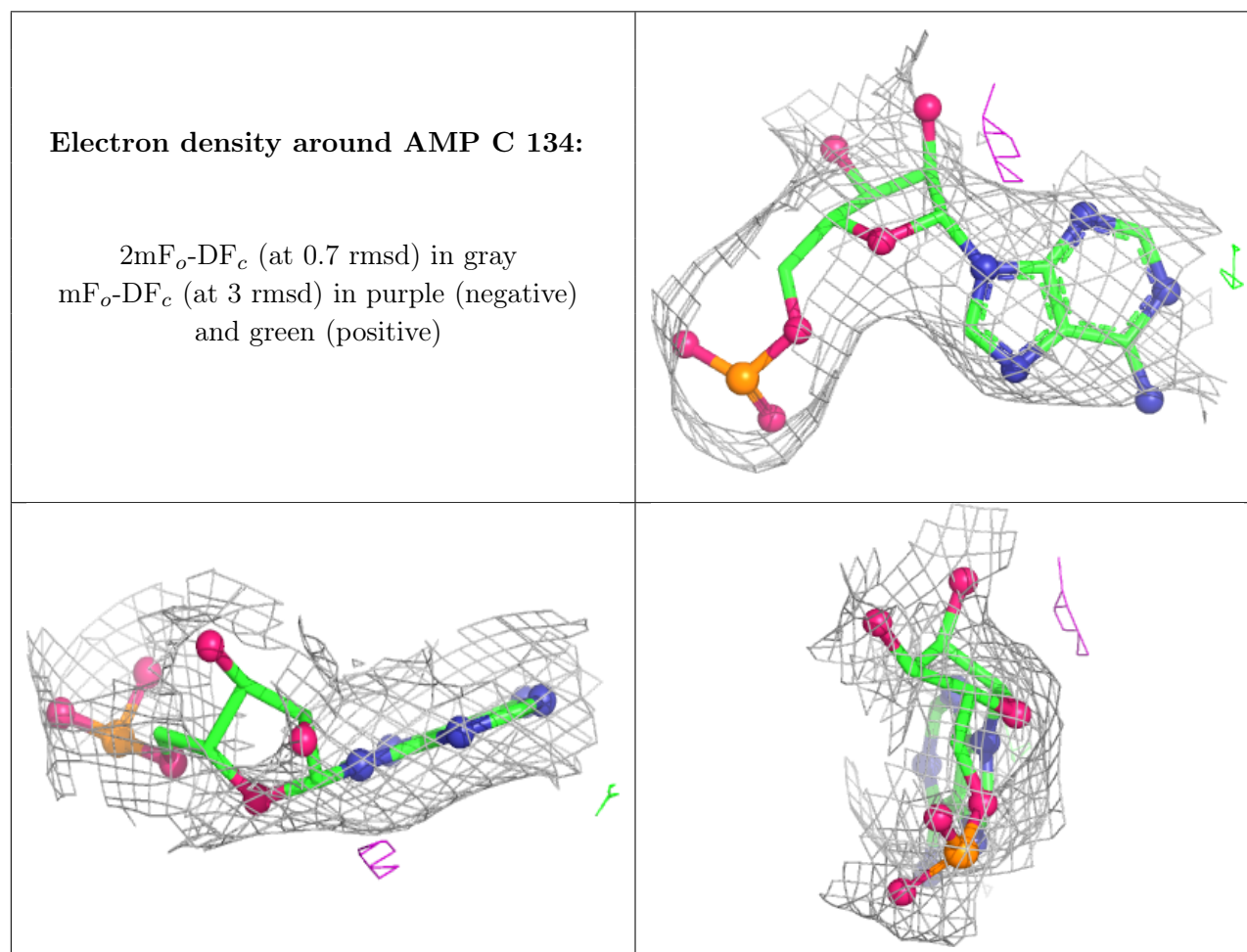
There are no oligosaccharides in this entry.

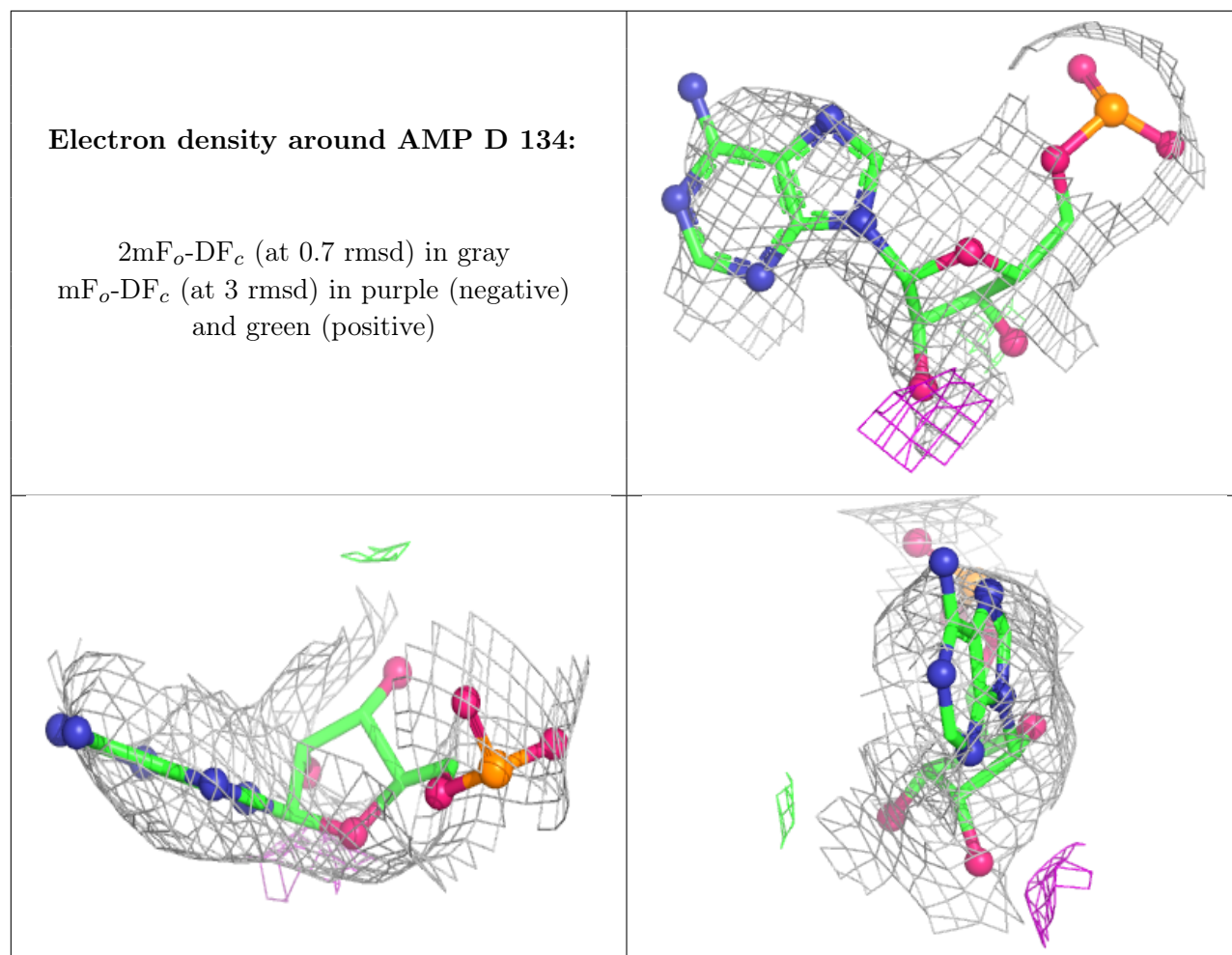
6.4 Ligands ⓘ

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	AMP	C	134	22/23	0.98	0.06	42,70,90,93	0
3	AMP	D	134	22/23	0.99	0.06	44,82,98,109	0
4	SO4	A	5001	5/5	0.99	0.03	46,53,60,63	0
4	SO4	B	5002	5/5	0.99	0.04	42,57,62,67	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.





6.5 Other polymers ⓘ

There are no such residues in this entry.