



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:48 am BST

PDB ID : 1EUQ  
Title : CRYSTAL STRUCTURE OF GLUTAMINYL-TRNA SYNTHETASE COM-  
PLEXED WITH A TRNA-GLN MUTANT AND AN ACTIVE-SITE IN-  
HIBITOR  
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Deposited on : 2000-04-17  
Resolution : 3.10 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

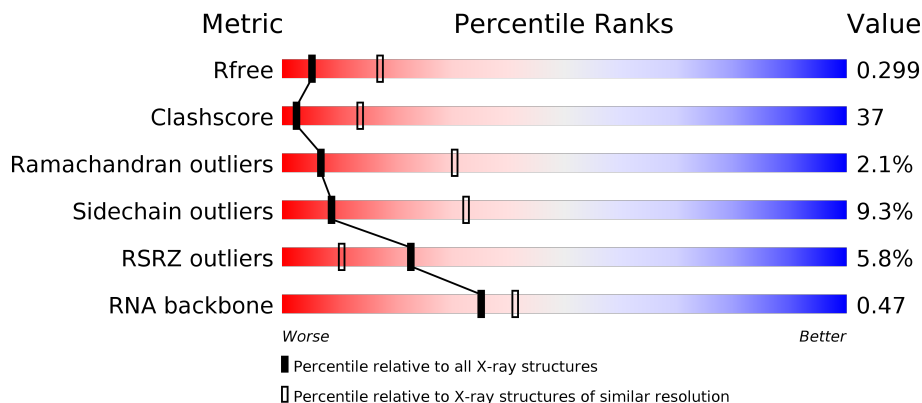
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	B	72	
2	A	548	

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	QSI	A	998	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5844 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.

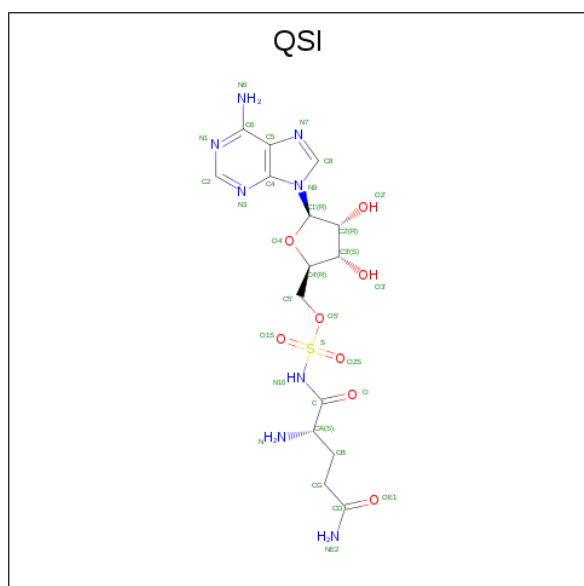
- Molecule 1 is a RNA chain called GLUTAMINYL TRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	B	72	Total	C	N	O	P	0	0	0
			1533	685	277	500	71			

- Molecule 2 is a protein called GLUTAMINYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	529	Total	C	N	O	S	0	0	0
			4279	2704	752	802	21			

- Molecule 3 is 5'-O-[N-(L-GLUTAMINYL)-SULFAMOYL]ADENOSINE (three-letter code: QSI) (formula: C<sub>15</sub>H<sub>22</sub>N<sub>8</sub>O<sub>8</sub>S).

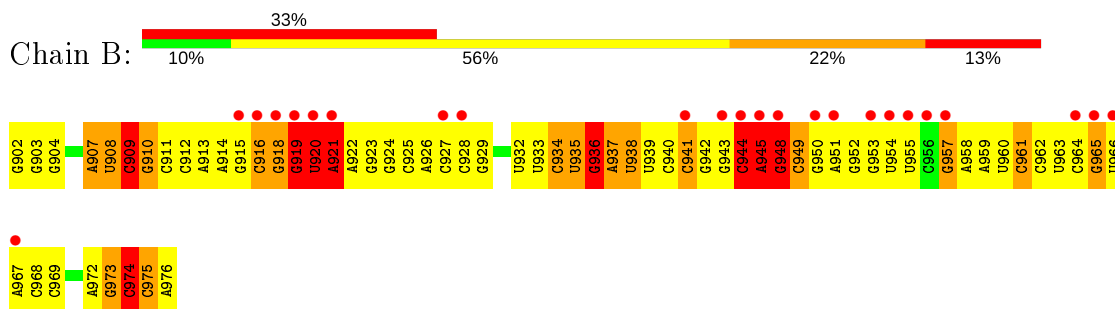


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	Total	C	N	O	S	0	0
			32	15	8	8	1		

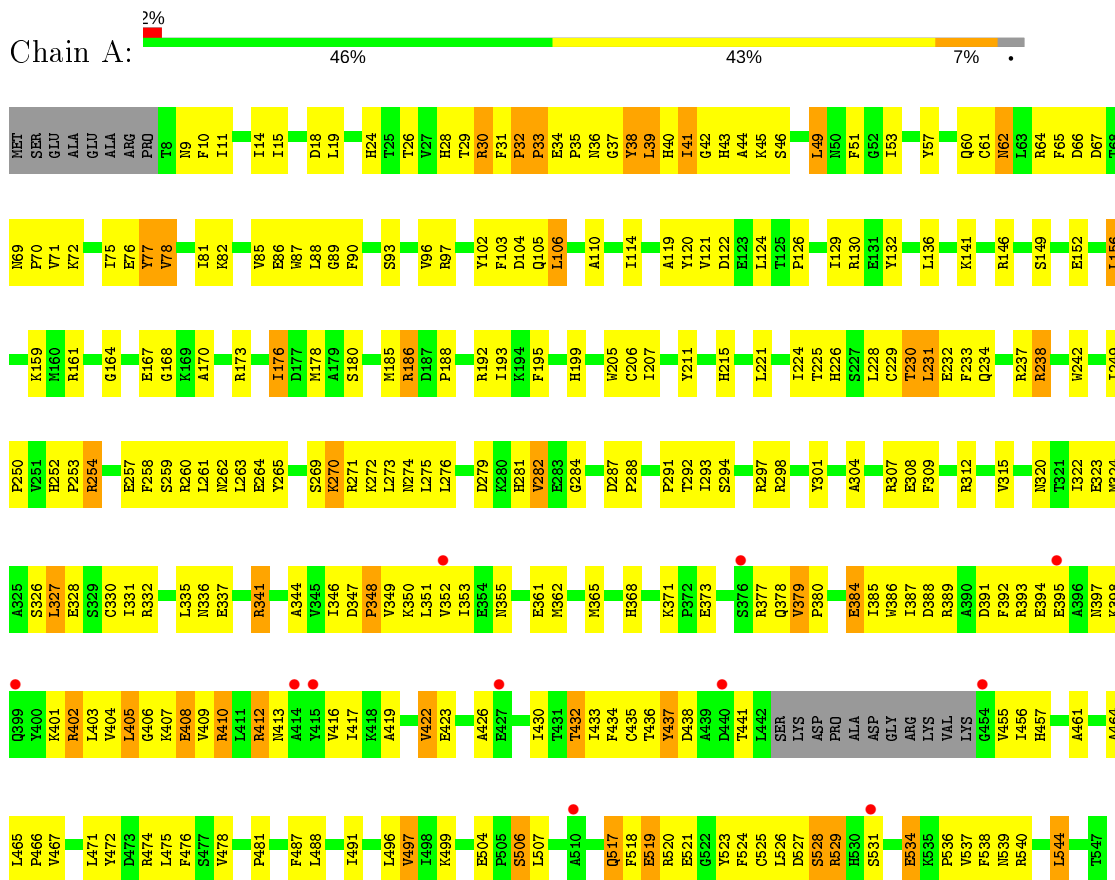
### 3 Residue-property plots

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

- Molecule 1: GLUTAMINYL TRNA



- Molecule 2: GLUTAMINYL-TRNA SYNTHETASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	230.91Å 93.59Å 113.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.10 30.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.10) 100.0 (30.00-3.10)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.96 (at 3.11Å)	Xtrriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.242 , 0.285 0.278 , 0.299	Depositor DCC
$R_{free}$ test set	2271 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.8	Xtrriage
Anisotropy	0.296	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 76.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	5844	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality i

### 5.1 Standard geometry i

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

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	B	1.23	17/1713 (1.0%)	1.24	22/2669 (0.8%)
2	A	0.58	0/4379	0.78	2/5928 (0.0%)
All	All	0.81	17/6092 (0.3%)	0.95	24/8597 (0.3%)

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	B	1	3
2	A	0	2
All	All	1	5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	945	A	O5'-C5'	18.47	1.74	1.44
1	B	945	A	C3'-O3'	16.76	1.65	1.42
1	B	945	A	C4'-C3'	16.65	1.71	1.53
1	B	948	G	O5'-C5'	14.74	1.68	1.44
1	B	945	A	C5'-C4'	13.89	1.68	1.51
1	B	945	A	P-O5'	12.26	1.72	1.59
1	B	948	G	C5'-C4'	10.36	1.63	1.51
1	B	945	A	O3'-P	7.50	1.70	1.61
1	B	948	G	C4'-C3'	7.34	1.61	1.53
1	B	945	A	C2'-O2'	7.00	1.50	1.41
1	B	945	A	P-OP2	6.19	1.59	1.49
1	B	948	G	P-OP2	-5.95	1.38	1.49
1	B	948	G	O3'-P	5.64	1.68	1.61
1	B	948	G	C3'-O3'	5.64	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	944	C	C3'-O3'	5.49	1.49	1.42
1	B	945	A	N9-C4	-5.12	1.34	1.37
1	B	921	A	C6-N6	-5.06	1.29	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	948	G	C5'-C4'-C3'	16.77	142.83	116.00
1	B	948	G	O5'-P-OP1	-13.62	93.44	105.70
1	B	945	A	C2'-C3'-O3'	-12.71	81.55	109.50
1	B	945	A	C5'-C4'-C3'	12.11	135.37	116.00
1	B	945	A	O3'-P-O5'	11.80	126.43	104.00
1	B	945	A	O5'-P-OP2	11.54	124.55	110.70
1	B	945	A	N9-C1'-C2'	10.02	127.02	114.00
1	B	948	G	O5'-P-OP2	-9.26	97.36	105.70
1	B	945	A	C4'-C3'-O3'	8.46	129.93	113.00
2	A	527	ASP	CB-CG-OD1	-7.93	111.16	118.30
1	B	945	A	OP2-P-O3'	7.60	121.92	105.20
1	B	936	G	N9-C1'-C2'	7.26	123.44	114.00
1	B	945	A	P-O5'-C5'	7.07	132.21	120.90
1	B	948	G	P-O5'-C5'	6.74	131.68	120.90
1	B	919	G	N9-C1'-C2'	6.61	122.59	114.00
1	B	945	A	P-O3'-C3'	6.37	127.34	119.70
1	B	945	A	C4'-C3'-C2'	-5.84	96.76	102.60
1	B	957	G	N9-C1'-C2'	-5.79	105.63	112.00
1	B	909	C	N1-C1'-C2'	5.70	121.41	114.00
2	A	250	PRO	N-CA-C	5.60	126.65	112.10
1	B	920	U	N1-C1'-C2'	5.36	120.96	114.00
1	B	974	C	N1-C1'-C2'	5.34	120.94	114.00
1	B	948	G	OP1-P-O3'	5.23	116.72	105.20
1	B	945	A	O4'-C1'-N9	-5.11	104.11	108.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	948	G	C4'

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	528	SER	Mainchain
2	A	77	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	B	909	C	Sidechain
1	B	919	G	Sidechain
1	B	938	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	B	1533	0	781	159	0
2	A	4279	0	4172	251	0
3	A	32	0	22	12	0
All	All	5844	0	4975	396	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 37.

All (396) 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:B:945:A:C3'	1:B:945:A:O3'	1.65	1.44
1:B:948:G:C5'	1:B:948:G:O5'	1.68	1.40
1:B:945:A:O5'	1:B:945:A:C5'	1.74	1.35
1:B:945:A:C2'	1:B:945:A:O3'	2.06	1.03
2:A:362:MET:HG3	2:A:378:GLN:HG3	1.42	1.00
2:A:531:SER:HB3	2:A:537:VAL:H	1.29	0.97
2:A:391:ASP:HA	2:A:402:ARG:HD2	1.47	0.96
2:A:433:ILE:HG22	2:A:435:CYS:SG	2.09	0.91
2:A:529:ARG:HA	2:A:529:ARG:HE	1.32	0.91
2:A:229:CYS:SG	3:A:998:QSI:NE2	2.45	0.90
1:B:933:U:H2'	1:B:935:U:OP1	1.73	0.89
2:A:229:CYS:SG	3:A:998:QSI:CD	2.61	0.88
1:B:921:A:C2	1:B:945:A:C6	2.63	0.87
1:B:937:A:C2	1:B:938:U:H1'	2.11	0.85
2:A:229:CYS:SG	3:A:998:QSI:OE1	2.34	0.85
1:B:903:G:H2'	1:B:904:G:H8	1.42	0.85
2:A:419:ALA:HA	2:A:435:CYS:SG	2.18	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:229:CYS:HG	3:A:998:QSI:CD	1.95	0.80
1:B:940:C:H2'	1:B:941:C:C6	2.18	0.78
2:A:102:TYR:O	2:A:106:LEU:HD22	1.83	0.78
1:B:916:C:H3'	1:B:916:C:OP2	1.83	0.78
2:A:176:ILE:HG13	2:A:188:PRO:HD2	1.67	0.77
1:B:903:G:H2'	1:B:904:G:C8	2.19	0.77
2:A:403:LEU:HD13	2:A:409:VAL:HG22	1.64	0.76
1:B:909:C:H5'	1:B:910:G:OP2	1.84	0.76
1:B:921:A:N6	1:B:948:G:OP2	2.19	0.75
1:B:916:C:H5''	1:B:918:G:H5''	1.70	0.74
1:B:972:A:C8	2:A:136:LEU:HD21	2.23	0.73
2:A:64:ARG:HA	2:A:97:ARG:O	1.89	0.73
2:A:347:ASP:O	2:A:388:ASP:HA	1.89	0.73
1:B:908:U:H5'	1:B:949:C:OP2	1.89	0.73
2:A:394:GLU:HA	2:A:405:LEU:HB2	1.71	0.72
1:B:949:C:O2'	1:B:950:G:H5'	1.89	0.72
2:A:471:LEU:HB2	2:A:497:VAL:HG13	1.70	0.72
1:B:918:G:C2	1:B:957:G:C6	2.77	0.72
1:B:976:A:H4'	2:A:34:GLU:OE1	1.90	0.72
1:B:961:C:H2'	1:B:962:C:C6	2.25	0.72
1:B:934:C:H5''	1:B:935:U:OP1	1.89	0.71
1:B:935:U:C5	1:B:937:A:C2	2.78	0.71
2:A:39:LEU:HD13	2:A:81:ILE:HG12	1.71	0.71
2:A:531:SER:HB3	2:A:537:VAL:N	2.02	0.71
1:B:948:G:O2'	1:B:949:C:P	2.49	0.70
2:A:341:ARG:HD2	2:A:341:ARG:H	1.56	0.70
2:A:40:HIS:HA	2:A:292:THR:HA	1.74	0.69
2:A:518:PHE:HZ	2:A:538:PHE:CD2	2.10	0.69
2:A:528:SER:O	2:A:529:ARG:NE	2.24	0.69
2:A:126:PRO:O	2:A:129:ILE:HG22	1.92	0.69
2:A:341:ARG:HD2	2:A:341:ARG:N	2.07	0.69
2:A:132:TYR:CD2	2:A:141:LYS:HG3	2.27	0.68
1:B:961:C:H2'	1:B:962:C:H6	1.58	0.68
2:A:529:ARG:NE	2:A:529:ARG:HA	2.08	0.68
2:A:534:GLU:O	2:A:536:PRO:HD3	1.94	0.68
1:B:919:G:O2'	1:B:920:U:H6	1.77	0.68
1:B:935:U:O2	2:A:519:GLU:HG3	1.93	0.68
1:B:950:G:O2'	1:B:951:A:H5'	1.93	0.68
1:B:944:C:OP2	1:B:944:C:C6	2.47	0.67
2:A:231:LEU:CD2	2:A:259:SER:HA	2.25	0.67
1:B:955:U:H1'	1:B:957:G:N7	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:933:U:H2'	1:B:935:U:P	2.35	0.66
2:A:176:ILE:HG21	2:A:185:MET:HB3	1.77	0.66
1:B:918:G:H5''	1:B:919:G:OP1	1.95	0.66
1:B:919:G:C4	1:B:957:G:N2	2.65	0.65
2:A:362:MET:CG	2:A:378:GLN:HG3	2.21	0.65
1:B:903:G:O2'	1:B:904:G:H5'	1.95	0.65
2:A:81:ILE:O	2:A:85:VAL:HG23	1.97	0.65
1:B:959:A:C5	1:B:960:U:C5	2.85	0.65
2:A:346:ILE:HD12	2:A:346:ILE:N	2.11	0.65
1:B:918:G:O2'	1:B:957:G:N2	2.27	0.65
1:B:918:G:C2	1:B:957:G:C5	2.86	0.64
1:B:958:A:C8	1:B:961:C:N4	2.66	0.64
2:A:526:LEU:HD12	2:A:537:VAL:O	1.98	0.64
1:B:909:C:C6	1:B:945:A:C2	2.85	0.64
2:A:309:PHE:CE1	2:A:322:ILE:HG21	2.33	0.64
2:A:129:ILE:HG13	2:A:173:ARG:NH2	2.13	0.64
2:A:28:HIS:HE1	2:A:62:ASN:OD1	1.80	0.64
2:A:433:ILE:HG22	2:A:435:CYS:HG	1.63	0.64
2:A:457:HIS:HD2	2:A:520:ARG:HE	1.45	0.63
1:B:937:A:H2'	1:B:938:U:O4'	1.98	0.63
1:B:919:G:O2'	1:B:920:U:C6	2.52	0.63
1:B:916:C:H5'	1:B:960:U:O2	1.99	0.63
2:A:159:LYS:HG2	2:A:164:GLY:HA3	1.81	0.63
2:A:394:GLU:HB3	2:A:405:LEU:HD22	1.81	0.62
2:A:353:ILE:HA	2:A:435:CYS:O	1.99	0.62
1:B:926:A:C2'	1:B:927:C:H5'	2.30	0.62
2:A:122:ASP:OD1	2:A:124:LEU:HD13	2.00	0.61
2:A:260:ARG:NH2	3:A:998:QSI:HN62	1.99	0.61
2:A:281:HIS:CE1	2:A:488:LEU:HD13	2.34	0.61
2:A:238:ARG:HD2	2:A:238:ARG:N	2.15	0.61
1:B:967:A:H2'	1:B:968:C:C6	2.35	0.60
2:A:403:LEU:HD13	2:A:409:VAL:CG2	2.30	0.60
1:B:916:C:C5'	1:B:960:U:O2	2.50	0.60
2:A:30:ARG:HH12	2:A:215:HIS:CE1	2.20	0.60
2:A:379:VAL:HG12	2:A:380:PRO:HD2	1.84	0.60
2:A:33:PRO:HA	3:A:998:QSI:H5'1	1.84	0.59
1:B:926:A:H2'	1:B:927:C:H5'	1.84	0.59
2:A:265:TYR:CD1	2:A:474:ARG:HD3	2.38	0.59
2:A:224:ILE:O	2:A:253:PRO:HB3	2.03	0.59
2:A:423:GLU:O	2:A:430:ILE:HG23	2.03	0.59
2:A:33:PRO:HD2	2:A:64:ARG:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:910:G:C6	1:B:926:A:C2	2.91	0.59
2:A:30:ARG:NH1	2:A:215:HIS:NE2	2.51	0.59
2:A:262:ASN:HB2	2:A:320:ASN:O	2.03	0.58
2:A:263:LEU:HD23	2:A:322:ILE:O	2.03	0.58
2:A:265:TYR:CG	2:A:474:ARG:HD3	2.38	0.58
1:B:958:A:C4	1:B:961:C:C5	2.91	0.58
2:A:309:PHE:CZ	2:A:322:ILE:HG21	2.39	0.58
2:A:422:VAL:HG22	2:A:423:GLU:H	1.69	0.58
2:A:393:ARG:O	2:A:404:VAL:HA	2.04	0.58
2:A:119:ALA:HA	2:A:173:ARG:O	2.03	0.58
2:A:386:TRP:CD1	2:A:461:ALA:HA	2.39	0.58
2:A:71:VAL:HG23	2:A:72:LYS:HG2	1.85	0.58
1:B:955:U:H3'	1:B:955:U:H6	1.69	0.58
1:B:907:A:C2	1:B:967:A:C2	2.92	0.57
1:B:908:U:N3	1:B:913:A:C6	2.73	0.57
2:A:231:LEU:HD22	2:A:259:SER:HA	1.85	0.57
2:A:284:GLY:H	2:A:287:ASP:HB2	1.70	0.57
2:A:301:TYR:CE2	2:A:327:LEU:HD22	2.39	0.57
2:A:518:PHE:CZ	2:A:538:PHE:CD2	2.91	0.57
1:B:903:G:C2	1:B:904:G:C4	2.93	0.57
2:A:44:ALA:HB2	2:A:293:ILE:HD11	1.87	0.56
1:B:935:U:O4	2:A:341:ARG:NH1	2.39	0.56
1:B:909:C:C5	1:B:945:A:C2	2.93	0.56
1:B:918:G:N2	1:B:957:G:C4	2.73	0.56
2:A:49:LEU:HG	2:A:315:VAL:HG21	1.88	0.56
2:A:167:GLU:HG3	2:A:195:PHE:CD2	2.41	0.55
2:A:478:VAL:O	2:A:481:PRO:HD3	2.05	0.55
2:A:504:GLU:OE2	2:A:506:SER:HB3	2.06	0.55
1:B:934:C:H4'	2:A:455:VAL:HG21	1.89	0.55
1:B:916:C:H4'	1:B:918:G:H5'	1.88	0.55
1:B:939:U:O2'	1:B:940:C:H5'	2.06	0.55
1:B:909:C:C5	1:B:945:A:N1	2.74	0.55
1:B:965:G:H2'	1:B:966:U:H6	1.72	0.55
1:B:953:G:O2'	1:B:954:U:H5'	2.07	0.55
2:A:132:TYR:HD2	2:A:141:LYS:O	1.90	0.55
2:A:365:MET:HG2	2:A:413:ASN:CB	2.37	0.55
2:A:271:ARG:O	2:A:274:ASN:HB3	2.08	0.54
2:A:351:LEU:HD11	2:A:417:ILE:HD12	1.89	0.54
2:A:207:ILE:HG13	2:A:207:ILE:O	2.07	0.54
2:A:39:LEU:HA	2:A:43:HIS:ND1	2.23	0.54
1:B:957:G:H2'	1:B:958:A:C5'	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:965:G:O2'	1:B:966:U:H5'	2.06	0.54
2:A:229:CYS:O	2:A:257:GLU:HA	2.07	0.54
1:B:948:G:HO2'	1:B:949:C:P	2.29	0.54
2:A:335:LEU:HB3	2:A:523:TYR:CD1	2.43	0.54
2:A:346:ILE:CG2	2:A:499:LYS:HG3	2.38	0.54
2:A:346:ILE:CD1	2:A:521:GLU:HG3	2.37	0.53
2:A:351:LEU:HD23	2:A:351:LEU:O	2.08	0.53
1:B:957:G:H2'	1:B:958:A:O5'	2.09	0.53
2:A:521:GLU:C	2:A:544:LEU:HD12	2.29	0.53
2:A:90:PHE:CZ	2:A:307:ARG:HD3	2.44	0.53
2:A:350:LYS:O	2:A:432:THR:HA	2.09	0.53
2:A:33:PRO:HA	3:A:998:QSI:C5'	2.39	0.53
2:A:120:TYR:CE2	2:A:146:ARG:HA	2.44	0.53
2:A:176:ILE:HB	2:A:185:MET:O	2.08	0.53
2:A:341:ARG:CZ	2:A:368:HIS:CE1	2.92	0.53
2:A:433:ILE:CG2	2:A:435:CYS:SG	2.91	0.53
2:A:53:ILE:O	2:A:57:TYR:HD1	1.91	0.53
2:A:206:CYS:SG	2:A:207:ILE:HG23	2.48	0.53
1:B:916:C:H4'	1:B:960:U:O2	2.07	0.53
1:B:911:C:H6	1:B:911:C:O5'	1.92	0.52
2:A:346:ILE:HD13	2:A:521:GLU:OE1	2.09	0.52
1:B:951:A:C6	1:B:952:G:C5	2.98	0.52
1:B:976:A:H3'	2:A:211:TYR:HB2	1.91	0.52
2:A:410:ARG:HD3	2:A:416:VAL:CG2	2.40	0.52
2:A:404:VAL:O	2:A:406:GLY:N	2.42	0.52
1:B:937:A:C2	1:B:938:U:C1'	2.87	0.52
1:B:916:C:O2'	1:B:918:G:OP2	2.25	0.52
2:A:42:GLY:O	2:A:45:LYS:HB3	2.09	0.52
2:A:301:TYR:CE2	2:A:331:ILE:HB	2.45	0.52
1:B:958:A:C8	1:B:961:C:C4	2.97	0.52
1:B:968:C:O2'	1:B:969:C:H5'	2.10	0.51
2:A:36:ASN:OD1	2:A:270:LYS:HD2	2.10	0.51
1:B:921:A:C2	1:B:945:A:N1	2.79	0.51
2:A:465:LEU:O	2:A:467:VAL:HG23	2.10	0.51
2:A:51:PHE:CD1	2:A:90:PHE:HB3	2.46	0.51
2:A:167:GLU:HG3	2:A:195:PHE:HD2	1.74	0.51
2:A:347:ASP:HB3	2:A:389:ARG:HD2	1.92	0.51
2:A:365:MET:HG2	2:A:413:ASN:HB3	1.93	0.51
2:A:412:ARG:HB2	2:A:457:HIS:HA	1.92	0.51
2:A:529:ARG:CA	2:A:529:ARG:HE	2.16	0.51
1:B:959:A:C4	1:B:960:U:C6	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:472:TYR:HE2	2:A:539:ASN:OD1	1.94	0.50
1:B:973:G:OP2	2:A:130:ARG:HD3	2.11	0.50
1:B:974:C:N3	2:A:168:GLY:HA2	2.26	0.50
2:A:237:ARG:NH1	2:A:257:GLU:OE1	2.44	0.50
2:A:28:HIS:HA	2:A:60:GLN:O	2.12	0.50
2:A:464:ALA:O	2:A:466:PRO:HD3	2.11	0.50
2:A:65:PHE:HE2	2:A:96:VAL:HG11	1.76	0.50
3:A:998:QSI:OE1	3:A:998:QSI:O3'	2.30	0.50
1:B:963:U:H2'	1:B:964:C:C6	2.46	0.50
2:A:103:PHE:HD2	2:A:205:TRP:CD1	2.30	0.50
2:A:149:SER:OG	2:A:152:GLU:HG3	2.11	0.50
2:A:230:THR:HG21	2:A:260:ARG:HB3	1.94	0.50
2:A:69:ASN:OD1	2:A:71:VAL:HG22	2.11	0.50
1:B:951:A:N1	1:B:964:C:N3	2.59	0.50
1:B:952:G:H2'	1:B:953:G:H8	1.76	0.50
2:A:178:MET:O	2:A:186:ARG:HD2	2.12	0.49
1:B:916:C:C4'	1:B:960:U:O2	2.60	0.49
2:A:476:PHE:CE1	2:A:491:ILE:HG12	2.47	0.49
1:B:967:A:C2	1:B:968:C:C2	3.00	0.49
2:A:270:LYS:O	2:A:274:ASN:HB2	2.11	0.49
2:A:42:GLY:HA2	2:A:261:LEU:HD23	1.94	0.49
2:A:40:HIS:O	2:A:43:HIS:N	2.45	0.49
1:B:902:G:N3	1:B:902:G:H2'	2.27	0.49
1:B:950:G:H2'	1:B:951:A:H8	1.77	0.49
2:A:384:GLU:O	2:A:461:ALA:HB3	2.13	0.49
2:A:230:THR:HB	2:A:232:GLU:OE1	2.12	0.49
2:A:404:VAL:HB	2:A:407:LYS:HB2	1.93	0.49
1:B:907:A:N1	1:B:967:A:C6	2.81	0.49
2:A:346:ILE:HD13	2:A:521:GLU:HG3	1.93	0.49
1:B:976:A:C2	2:A:233:PHE:CE1	3.01	0.49
2:A:392:PHE:CE2	2:A:430:ILE:HD13	2.48	0.48
2:A:412:ARG:NH1	2:A:412:ARG:HG2	2.29	0.48
2:A:525:CYS:O	2:A:539:ASN:N	2.44	0.48
2:A:534:GLU:H	2:A:534:GLU:CD	2.17	0.48
1:B:909:C:C5'	1:B:910:G:OP2	2.59	0.48
1:B:950:G:H2'	1:B:951:A:O4'	2.13	0.48
2:A:517:GLN:HG3	2:A:523:TYR:CE1	2.49	0.48
1:B:932:U:C4	1:B:933:U:C5	3.02	0.48
1:B:936:G:OP2	2:A:401:LYS:HE3	2.14	0.48
1:B:924:G:C6	1:B:925:C:C4	3.02	0.48
2:A:263:LEU:HD11	2:A:327:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:43:HIS:O	2:A:46:SER:N	2.47	0.48
2:A:322:ILE:N	2:A:322:ILE:CD1	2.77	0.47
2:A:408:GLU:HB3	2:A:417:ILE:O	2.14	0.47
1:B:916:C:H5'	1:B:960:U:C2	2.49	0.47
1:B:902:G:H1'	2:A:136:LEU:O	2.14	0.47
2:A:105:GLN:HA	2:A:105:GLN:OE1	2.12	0.47
2:A:455:VAL:HG12	2:A:456:ILE:N	2.29	0.47
2:A:75:ILE:O	2:A:78:VAL:HG13	2.15	0.47
1:B:951:A:N1	1:B:952:G:C5	2.82	0.47
2:A:392:PHE:CE2	2:A:430:ILE:CD1	2.97	0.47
2:A:309:PHE:HE1	2:A:322:ILE:HG21	1.80	0.47
2:A:341:ARG:NH1	2:A:368:HIS:CE1	2.83	0.47
2:A:60:GLN:HB3	2:A:93:SER:HB2	1.97	0.47
1:B:926:A:H2'	1:B:927:C:O4'	2.15	0.47
2:A:496:LEU:HD12	2:A:497:VAL:N	2.29	0.47
1:B:936:G:H3'	1:B:937:A:H5'	1.96	0.47
2:A:230:THR:HA	2:A:258:PHE:O	2.14	0.47
1:B:929:G:C6	1:B:942:G:C6	3.03	0.47
1:B:934:C:O2'	2:A:412:ARG:NH1	2.49	0.46
2:A:276:LEU:HB3	2:A:282:VAL:HG22	1.97	0.46
2:A:410:ARG:HD3	2:A:416:VAL:HG22	1.98	0.46
2:A:392:PHE:HE2	2:A:430:ILE:CD1	2.29	0.46
1:B:918:G:N2	1:B:957:G:C5	2.83	0.46
2:A:438:ASP:HB3	2:A:441:THR:OG1	2.15	0.46
2:A:471:LEU:HD12	2:A:497:VAL:HG22	1.97	0.46
2:A:346:ILE:HG22	2:A:499:LYS:HG3	1.98	0.46
1:B:965:G:H2'	1:B:966:U:C6	2.49	0.46
1:B:939:U:H2'	1:B:940:C:O4'	2.16	0.46
1:B:941:C:H2'	1:B:942:G:H8	1.81	0.46
1:B:972:A:N7	2:A:136:LEU:HD21	2.30	0.46
1:B:911:C:H2'	1:B:912:C:O5'	2.15	0.46
1:B:945:A:O3'	1:B:945:A:O2'	2.33	0.46
1:B:948:G:O2'	1:B:949:C:OP2	2.30	0.46
2:A:46:SER:CB	3:A:998:QSI:H1'	2.46	0.46
1:B:967:A:C6	1:B:968:C:N4	2.84	0.46
1:B:967:A:C2	1:B:968:C:N3	2.84	0.46
2:A:60:GLN:OE1	2:A:93:SER:HB2	2.16	0.45
1:B:918:G:N2	1:B:958:A:O5'	2.49	0.45
1:B:955:U:H3'	1:B:955:U:C6	2.50	0.45
2:A:264:GLU:O	2:A:265:TYR:HB2	2.15	0.45
2:A:301:TYR:CE2	2:A:327:LEU:CD2	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:346:ILE:N	2:A:346:ILE:CD1	2.79	0.45
2:A:351:LEU:HD22	2:A:385:ILE:HG12	1.98	0.45
2:A:407:LYS:HG3	2:A:408:GLU:H	1.82	0.45
2:A:412:ARG:HH11	2:A:412:ARG:HG2	1.82	0.45
2:A:10:PHE:O	2:A:14:ILE:HG13	2.16	0.45
1:B:950:G:C2	1:B:965:G:C2	3.05	0.45
2:A:528:SER:O	2:A:529:ARG:CZ	2.64	0.45
2:A:82:LYS:HB2	2:A:82:LYS:HE3	1.78	0.45
2:A:225:THR:OG1	2:A:226:HIS:HD2	2.00	0.45
1:B:903:G:C4	1:B:904:G:C8	3.05	0.45
2:A:41:ILE:O	2:A:44:ALA:HB3	2.17	0.45
2:A:336:ASN:O	2:A:341:ARG:NH2	2.50	0.45
2:A:352:VAL:HG23	2:A:434:PHE:HA	1.99	0.45
2:A:221:LEU:HG	2:A:249:ILE:HD11	1.98	0.44
1:B:953:G:C5	1:B:954:U:C5	3.05	0.44
2:A:110:ALA:O	2:A:114:ILE:HG13	2.16	0.44
1:B:919:G:C2	1:B:957:G:C2	3.05	0.44
1:B:918:G:N2	1:B:955:U:O2	2.47	0.44
2:A:38:TYR:CD1	2:A:38:TYR:N	2.86	0.44
2:A:105:GLN:HG2	2:A:221:LEU:HD13	2.00	0.44
2:A:322:ILE:HG22	2:A:323:GLU:O	2.16	0.44
1:B:932:U:C4	1:B:933:U:C4	3.05	0.44
1:B:907:A:C2	1:B:967:A:C4	3.06	0.44
1:B:904:G:H1	1:B:969:C:H42	1.64	0.44
2:A:35:PRO:HD3	2:A:65:PHE:HB3	1.98	0.44
1:B:975:C:H2'	1:B:976:A:O4'	2.17	0.44
1:B:974:C:O2'	1:B:975:C:P	2.75	0.44
1:B:976:A:C2	2:A:233:PHE:CZ	3.06	0.44
1:B:940:C:N3	1:B:941:C:N4	2.66	0.44
2:A:121:VAL:HG21	2:A:156:LEU:HB3	1.99	0.44
2:A:351:LEU:HD11	2:A:417:ILE:CD1	2.46	0.44
2:A:336:ASN:O	2:A:368:HIS:HE1	2.00	0.44
1:B:919:G:C2	1:B:957:G:N3	2.86	0.44
1:B:907:A:C2	1:B:967:A:N3	2.86	0.44
2:A:37:GLY:N	2:A:77:TYR:CD2	2.86	0.44
1:B:963:U:N3	1:B:964:C:C4	2.86	0.44
1:B:972:A:C5	2:A:136:LEU:HG	2.53	0.43
1:B:945:A:C3'	1:B:948:G:P	3.00	0.43
2:A:126:PRO:HA	2:A:129:ILE:HG22	1.99	0.43
2:A:301:TYR:CZ	2:A:327:LEU:HD22	2.53	0.43
2:A:30:ARG:HG2	2:A:32:PRO:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:377:ARG:HH11	2:A:377:ARG:HG2	1.83	0.43
1:B:926:A:H2'	1:B:927:C:C5'	2.48	0.43
2:A:78:VAL:O	2:A:82:LYS:HB2	2.18	0.43
1:B:918:G:C5'	1:B:919:G:OP1	2.66	0.43
1:B:950:G:H2'	1:B:951:A:C8	2.53	0.43
1:B:967:A:C5	1:B:968:C:C4	3.06	0.43
2:A:86:GLU:O	2:A:89:GLY:N	2.52	0.43
2:A:260:ARG:HH21	3:A:998:QSI:HN62	1.64	0.43
1:B:918:G:H4'	1:B:919:G:OP1	2.19	0.43
2:A:33:PRO:O	2:A:33:PRO:HG2	2.19	0.43
1:B:916:C:P	1:B:916:C:H3'	2.58	0.43
1:B:935:U:H5	1:B:937:A:C2	2.31	0.43
1:B:955:U:C3'	1:B:955:U:C6	3.02	0.43
2:A:351:LEU:HD23	2:A:351:LEU:C	2.39	0.43
2:A:234:GLN:HG2	2:A:257:GLU:CD	2.39	0.43
2:A:434:PHE:N	2:A:434:PHE:CD1	2.87	0.43
1:B:916:C:H3'	1:B:916:C:O2	2.19	0.43
2:A:275:LEU:HD11	2:A:279:ASP:OD2	2.19	0.43
2:A:525:CYS:SG	2:A:539:ASN:HB2	2.59	0.43
1:B:940:C:H2'	1:B:941:C:C5	2.51	0.43
1:B:951:A:C2	1:B:964:C:O2	2.72	0.43
2:A:346:ILE:HD12	2:A:346:ILE:H	1.84	0.43
2:A:398:LYS:HG2	2:A:398:LYS:O	2.17	0.43
2:A:524:PHE:N	2:A:524:PHE:CD1	2.87	0.43
1:B:928:C:C2	1:B:943:G:C2	3.07	0.43
2:A:331:ILE:HG23	2:A:332:ARG:N	2.34	0.42
2:A:349:VAL:HB	2:A:389:ARG:HG2	2.01	0.42
2:A:347:ASP:HB2	2:A:388:ASP:OD1	2.19	0.42
1:B:958:A:H3'	1:B:958:A:OP1	2.19	0.42
1:B:963:U:H2'	1:B:964:C:O4'	2.19	0.42
2:A:15:ILE:HD12	2:A:53:ILE:HD13	2.00	0.42
2:A:170:ALA:O	2:A:193:ILE:HD12	2.19	0.42
2:A:18:ASP:HB3	2:A:24:HIS:HD2	1.84	0.42
2:A:324:MET:O	2:A:328:GLU:HG3	2.19	0.42
1:B:944:C:H6	1:B:944:C:P	2.42	0.42
2:A:31:PHE:CD2	2:A:33:PRO:HD3	2.55	0.42
2:A:29:THR:O	2:A:61:CYS:HA	2.19	0.42
1:B:952:G:H2'	1:B:953:G:C8	2.55	0.42
1:B:976:A:H2'	3:A:998:QSI:HA	2.01	0.42
3:A:998:QSI:HB1	3:A:998:QSI:O3'	2.19	0.42
1:B:921:A:C2	1:B:945:A:N6	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:958:A:C5	1:B:961:C:C4	3.07	0.42
2:A:312:ARG:NH1	2:A:330:CYS:SG	2.93	0.42
2:A:355:ASN:HB2	2:A:436:THR:HG22	2.00	0.42
1:B:918:G:H21	1:B:958:A:C5'	2.33	0.42
2:A:269:SER:C	2:A:271:ARG:N	2.73	0.42
2:A:288:PRO:HG3	2:A:298:ARG:HG2	2.01	0.42
2:A:304:ALA:O	2:A:308:GLU:N	2.51	0.42
1:B:934:C:O2'	2:A:412:ARG:NH2	2.53	0.42
2:A:67:ASP:HB2	2:A:199:HIS:HE2	1.84	0.42
2:A:353:ILE:HD13	2:A:437:TYR:HB3	2.02	0.42
2:A:404:VAL:HB	2:A:407:LYS:CB	2.50	0.42
1:B:916:C:H4'	1:B:918:G:C5'	2.49	0.42
2:A:252:HIS:CE1	2:A:254:ARG:HH22	2.38	0.42
2:A:273:LEU:HD21	2:A:291:PRO:CG	2.50	0.42
2:A:337:GLU:OE2	2:A:371:LYS:HD2	2.19	0.42
1:B:904:G:H1	1:B:969:C:N4	2.18	0.42
2:A:403:LEU:CD1	2:A:409:VAL:HG13	2.50	0.41
1:B:914:A:N6	1:B:915:G:C2	2.88	0.41
1:B:957:G:H2'	1:B:958:A:H5'	2.01	0.41
2:A:234:GLN:HA	2:A:257:GLU:OE2	2.20	0.41
2:A:518:PHE:HZ	2:A:538:PHE:CE2	2.38	0.41
2:A:176:ILE:HD13	2:A:242:TRP:CE2	2.55	0.41
2:A:272:LYS:HB3	2:A:487:PHE:CE2	2.55	0.41
2:A:11:ILE:HD12	2:A:49:LEU:HD11	2.03	0.41
2:A:386:TRP:NE1	2:A:461:ALA:HA	2.36	0.41
2:A:471:LEU:HD22	2:A:540:ARG:NH1	2.36	0.41
2:A:534:GLU:C	2:A:536:PRO:HD3	2.41	0.41
1:B:918:G:H5'	1:B:960:U:O2	2.21	0.41
2:A:224:ILE:HD13	2:A:224:ILE:HA	1.89	0.41
2:A:344:ALA:O	2:A:457:HIS:CE1	2.73	0.41
1:B:910:G:C5	1:B:926:A:C2	3.09	0.41
2:A:269:SER:O	2:A:271:ARG:N	2.54	0.41
2:A:348:PRO:HA	2:A:387:ILE:O	2.21	0.41
2:A:38:TYR:HD1	2:A:38:TYR:N	2.19	0.41
2:A:273:LEU:HD21	2:A:291:PRO:HG3	2.02	0.41
1:B:902:G:N2	1:B:903:G:H1'	2.36	0.41
2:A:261:LEU:HD12	2:A:262:ASN:N	2.36	0.41
2:A:75:ILE:HG23	2:A:76:GLU:N	2.34	0.41
2:A:11:ILE:HD13	2:A:228:LEU:HD13	2.02	0.40
2:A:88:LEU:HB3	2:A:90:PHE:CE2	2.56	0.40
2:A:180:SER:O	2:A:186:ARG:NH1	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:9:ASN:OD1	2:A:9:ASN:C	2.59	0.40
1:B:919:G:N3	1:B:957:G:N2	2.69	0.40
2:A:87:TRP:NE1	2:A:297:ARG:HD3	2.36	0.40
1:B:943:G:H2'	1:B:944:C:OP2	2.21	0.40
2:A:377:ARG:NH1	2:A:377:ARG:HG2	2.35	0.40
2:A:433:ILE:HG22	2:A:433:ILE:O	2.22	0.40
2:A:70:PRO:HG2	2:A:71:VAL:H	1.87	0.40
1:B:914:A:C6	1:B:915:G:C2	3.10	0.40
1:B:923:G:C2	1:B:924:G:C8	3.10	0.40
1:B:951:A:N6	1:B:964:C:H42	2.19	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	525/548 (96%)	449 (86%)	65 (12%)	11 (2%)	<b>7</b> <b>30</b>

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	405	LEU
2	A	422	VAL
2	A	348	PRO
2	A	397	ASN
2	A	32	PRO
2	A	361	GLU
2	A	402	ARG
2	A	426	ALA
2	A	507	LEU
2	A	176	ILE
2	A	41	ILE

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	A	463/478 (97%)	420 (91%)	43 (9%)	9 32

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	19	LEU
2	A	26	THR
2	A	30	ARG
2	A	33	PRO
2	A	38	TYR
2	A	39	LEU
2	A	49	LEU
2	A	62	ASN
2	A	66	ASP
2	A	78	VAL
2	A	104	ASP
2	A	106	LEU
2	A	156	LEU
2	A	161	ARG
2	A	186	ARG
2	A	192	ARG
2	A	230	THR
2	A	231	LEU
2	A	238	ARG
2	A	254	ARG
2	A	270	LYS
2	A	282	VAL
2	A	294	SER
2	A	326	SER
2	A	327	LEU
2	A	341	ARG
2	A	373	GLU
2	A	379	VAL
2	A	384	GLU
2	A	395	GLU

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Mol	Chain	Res	Type
2	A	408	GLU
2	A	410	ARG
2	A	412	ARG
2	A	432	THR
2	A	437	TYR
2	A	475	LEU
2	A	497	VAL
2	A	506	SER
2	A	517	GLN
2	A	519	GLU
2	A	529	ARG
2	A	534	GLU
2	A	544	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	24	HIS
2	A	28	HIS
2	A	142	ASN
2	A	153	ASN
2	A	226	HIS
2	A	236	ASN
2	A	246	ASN
2	A	281	HIS
2	A	355	ASN
2	A	368	HIS
2	A	457	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	71/72 (98%)	20 (28%)	13 (18%)

All (20) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	908	U
1	B	909	C
1	B	910	G

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Mol	Chain	Res	Type
1	B	916	C
1	B	918	G
1	B	919	G
1	B	921	A
1	B	922	A
1	B	935	U
1	B	936	G
1	B	937	A
1	B	941	C
1	B	944	C
1	B	945	A
1	B	948	G
1	B	949	C
1	B	961	C
1	B	965	G
1	B	973	G
1	B	975	C

All (13) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	907	A
1	B	909	C
1	B	916	C
1	B	918	G
1	B	919	G
1	B	920	U
1	B	934	C
1	B	935	U
1	B	936	G
1	B	945	A
1	B	948	G
1	B	973	G
1	B	974	C

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	QSI	A	998	-	31,34,34	3.32	6 (19%)	34,50,50	0.98	2 (5%)

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	QSI	A	998	-	-	7/19/40/40	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	998	QSI	O1S-S	12.76	1.53	1.42
3	A	998	QSI	S-N10	9.35	1.76	1.59
3	A	998	QSI	O2S-S	5.24	1.46	1.42
3	A	998	QSI	O5'-S	-5.19	1.48	1.59
3	A	998	QSI	CD-NE2	4.26	1.46	1.32
3	A	998	QSI	CA-N	-2.91	1.33	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	998	QSI	C-N10-S	-2.51	120.54	124.61
3	A	998	QSI	C5-C6-N6	2.30	123.85	120.35

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	998	QSI	O-C-N10-S
3	A	998	QSI	C-N10-S-O1S
3	A	998	QSI	C-N10-S-O2S
3	A	998	QSI	N-CA-CB-CG
3	A	998	QSI	N10-C-CA-CB
3	A	998	QSI	O-C-CA-N
3	A	998	QSI	C-CA-CB-CG

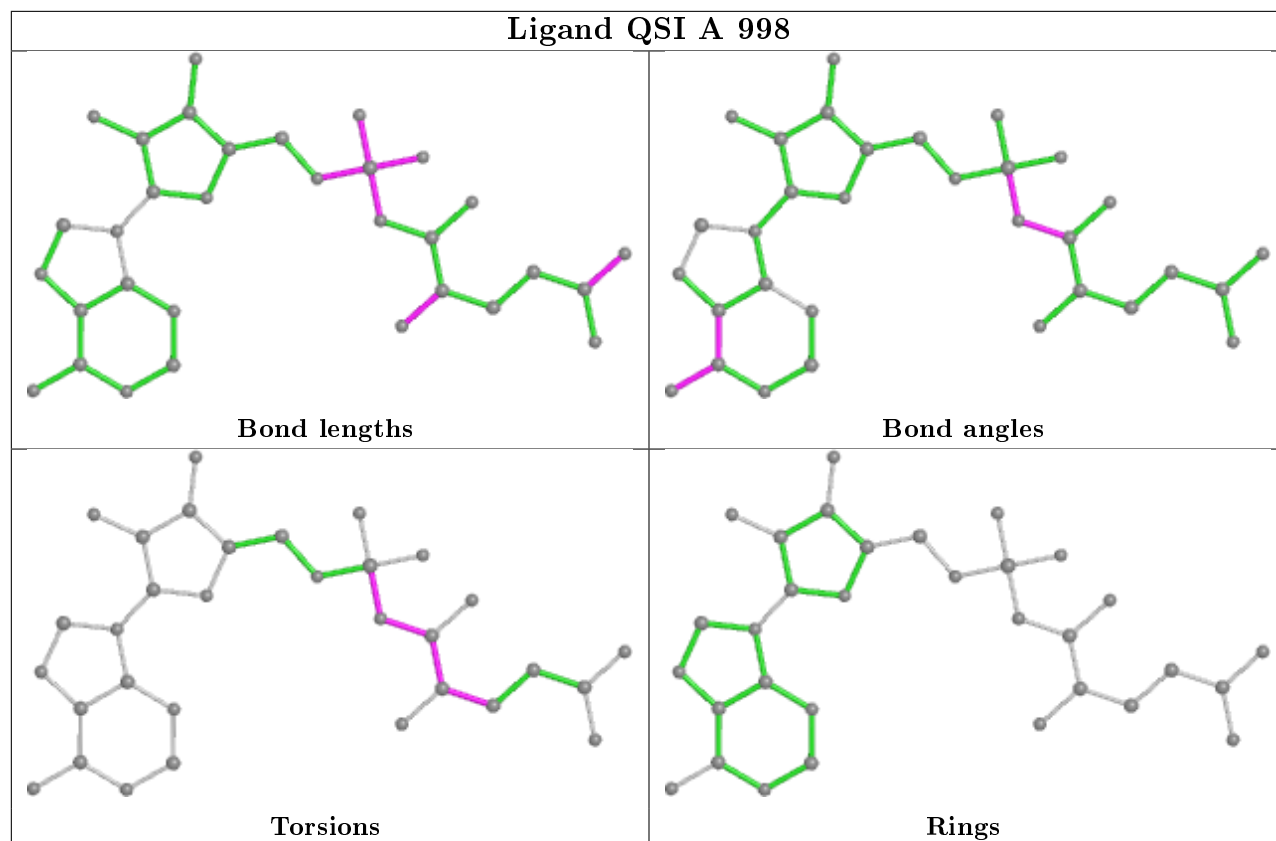
There are no ring outliers.

1 monomer is involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	998	QSI	12	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	B	72/72 (100%)	1.49	24 (33%) 0 0	0, 57, 87, 94	0
2	A	529/548 (96%)	-0.07	11 (2%) 63 43	3, 24, 65, 91	0
All	All	601/620 (96%)	0.12	35 (5%) 23 10	0, 27, 74, 94	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	916	C	5.7
1	B	953	G	5.0
1	B	955	U	4.9
1	B	956	C	4.4
1	B	915	G	4.1
1	B	920	U	4.0
1	B	957	G	3.8
1	B	919	G	3.7
1	B	944	C	3.5
1	B	954	U	3.4
1	B	945	A	3.1
2	A	427	GLU	2.9
1	B	918	G	2.9
1	B	927	C	2.7
1	B	941	C	2.7
1	B	948	G	2.7
2	A	510	ALA	2.5
2	A	399	GLN	2.4
1	B	951	A	2.4
2	A	454	GLY	2.4
1	B	950	G	2.3
1	B	966	U	2.3
2	A	440	ASP	2.3
2	A	376	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	965	G	2.3
1	B	964	C	2.3
2	A	352	VAL	2.2
1	B	967	A	2.2
1	B	943	G	2.1
2	A	531	SER	2.1
2	A	395	GLU	2.1
1	B	921	A	2.1
1	B	928	C	2.0
2	A	414	ALA	2.0
2	A	415	TYR	2.0

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

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

## 6.3 Carbohydrates [i](#)

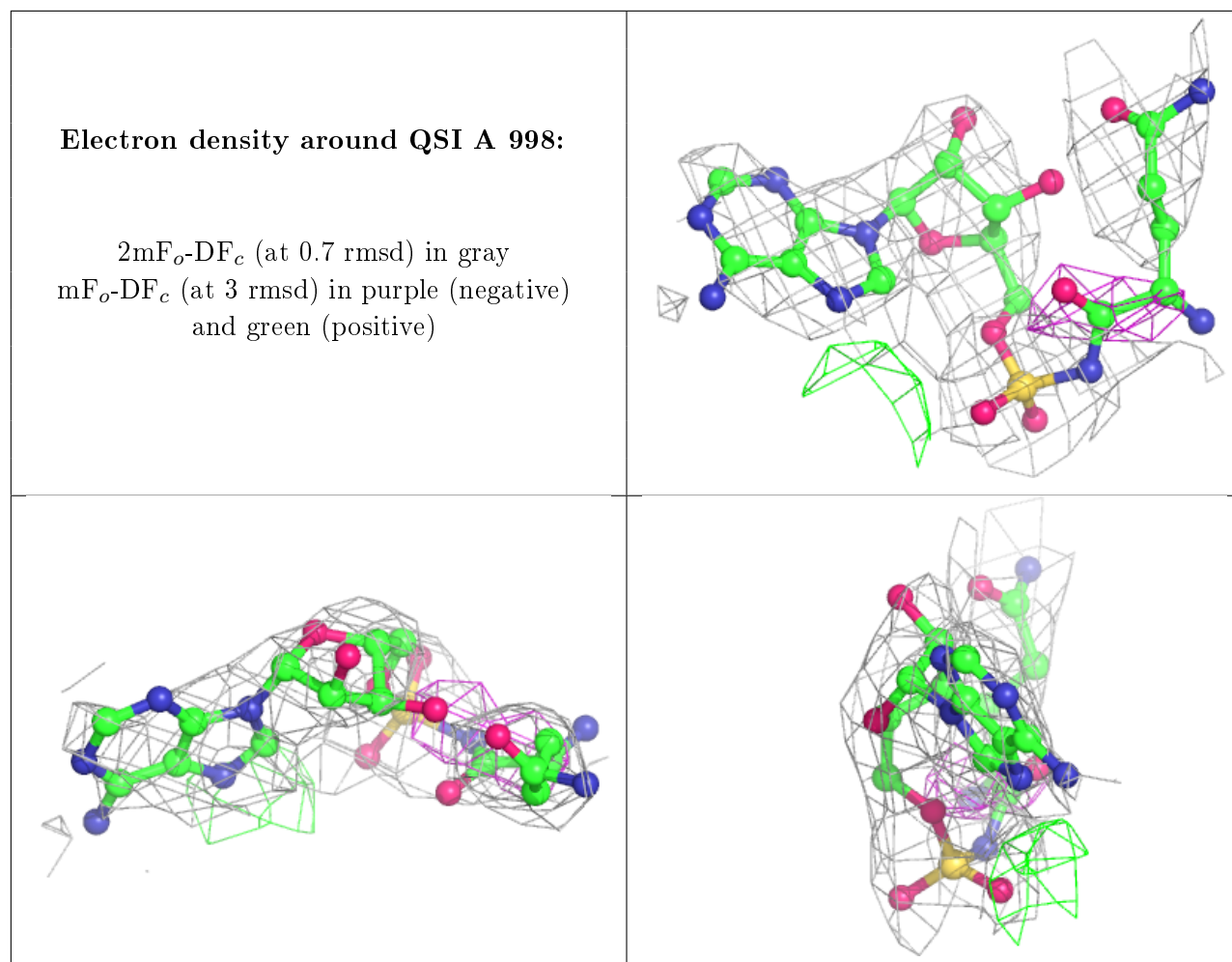
There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	QSI	A	998	32/32	0.90	0.26	12,51,60,62	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 [i](#)

There are no such residues in this entry.