



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 09:57 PM EDT

PDB ID : 1EUY / pdb_00001euy
Title : GLUTAMINYL-TRNA SYNTHETASE COMPLEXED WITH A TRNA MUTANT AND AN ACTIVE SITE INHIBITOR
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Deposited on : 2000-04-19
Resolution : 2.60 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

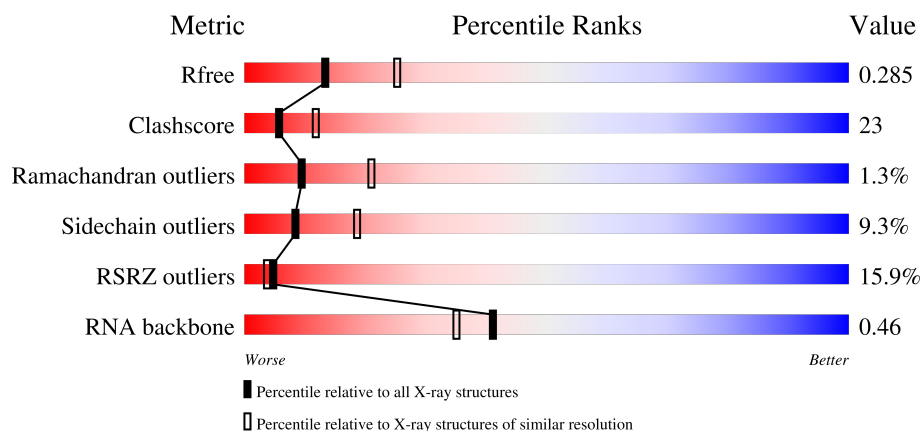
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)
RNA backbone	3983	1014 (2.84-2.36)

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	B	74	
2	A	548	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5915 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.

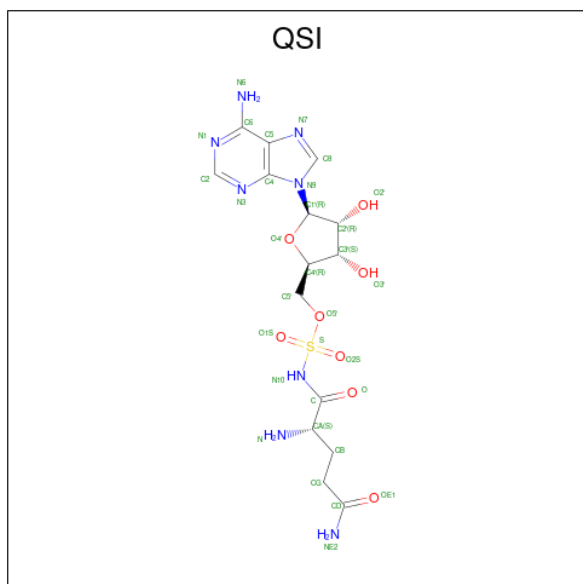
- Molecule 1 is a RNA chain called GLUTAMINYL TRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	73	Total	C	N	O	P	0	0	0
			1555	695	282	506	72			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	529	Total	C	N	O	S	0	0	0
			4274	2701	751	801	21			

- Molecule 3 is 5'-O-[N-(L-GLUTAMINYL)-SULFAMOYL]ADENOSINE (CCD ID: QSI) (formula: C₁₅H₂₂N₈O₈S).



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

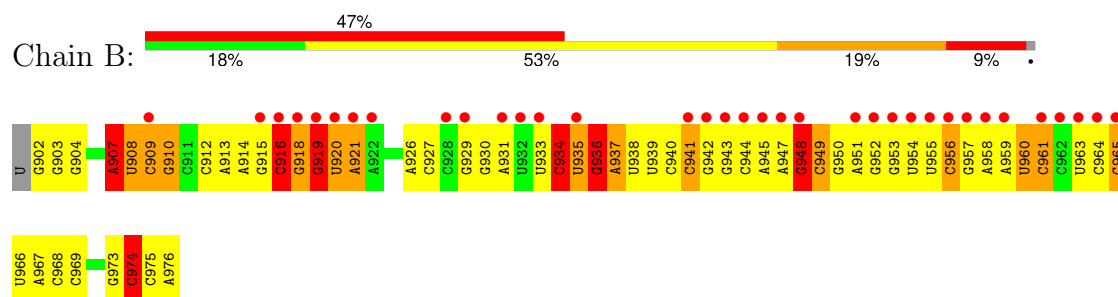
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	18	Total 18	O 18	0	0
4	A	36	Total 36	O 36	0	0

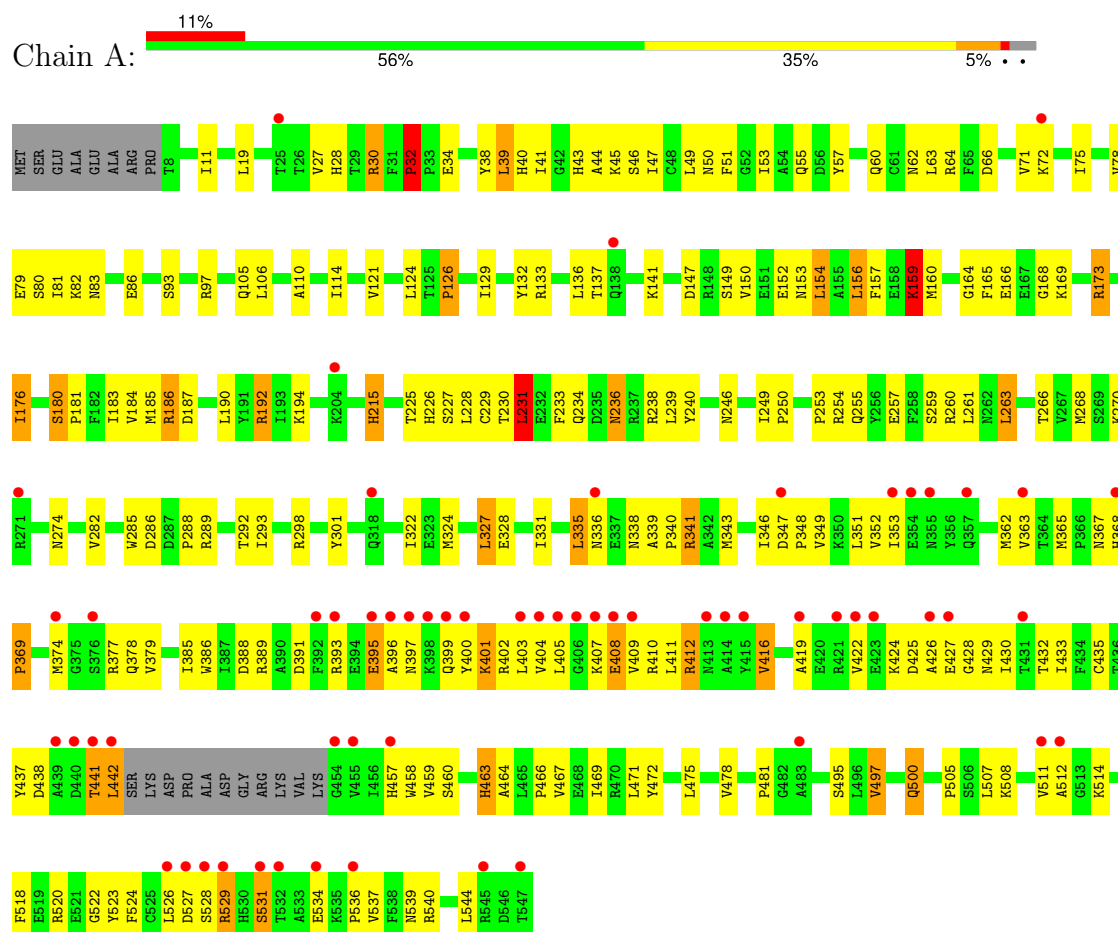
3 Residue-property plots [i](#)

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

• Molecule 1: 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, α , β , γ	235.20Å 94.20Å 113.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 30.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.5 (30.00-2.60) 98.7 (30.00-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.45Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.234 , 0.277 0.288 , 0.285	Depositor DCC
R_{free} test set	4626 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 66.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	5915	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: 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	0.45	0/1738	0.85	8/2708 (0.3%)
2	A	0.63	0/4374	1.04	19/5921 (0.3%)
All	All	0.58	0/6112	0.98	27/8629 (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	0	4

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	215	HIS	N-CA-C	9.49	121.63	111.28
2	A	246	ASN	N-CA-C	7.42	122.04	112.92
2	A	250	PRO	N-CA-C	7.17	122.85	114.03
2	A	401	LYS	N-CA-C	7.13	121.81	113.18
1	B	919	G	N9-C1'-C2'	6.62	121.93	112.00
2	A	63	LEU	N-CA-C	-6.55	97.74	108.41
2	A	339	ALA	N-CA-C	6.32	117.62	109.65
2	A	147	ASP	N-CA-C	6.27	119.87	112.72
2	A	518	PHE	N-CA-C	-6.07	98.63	108.41
1	B	919	G	C4'-C3'-O3'	-6.02	103.97	113.00
2	A	32	PRO	N-CA-C	6.01	118.04	110.70
2	A	181	PRO	N-CA-C	-6.01	105.83	114.18
1	B	974	C	N1-C1'-C2'	5.87	122.80	114.00
1	B	936	G	N9-C1'-C2'	5.77	122.66	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	249	ILE	CA-C-N	5.76	125.86	119.87
2	A	249	ILE	C-N-CA	5.76	125.86	119.87
1	B	934	C	N1-C1'-C2'	5.74	122.60	114.00
2	A	231	LEU	N-CA-C	5.71	118.28	111.71
1	B	948	G	C2'-C3'-O3'	5.40	117.61	109.50
1	B	916	C	C2'-C3'-O3'	5.40	117.60	109.50
2	A	500	GLN	N-CA-C	-5.22	100.01	108.52
2	A	338	ASN	N-CA-C	5.18	119.69	112.90
1	B	974	C	C4'-C3'-O3'	-5.18	101.63	109.40
2	A	133	ARG	N-CA-C	5.18	118.86	112.54
2	A	159	LYS	N-CA-C	-5.15	105.67	111.28
2	A	34	GLU	N-CA-C	-5.11	103.59	109.93
2	A	416	VAL	N-CA-C	-5.01	101.36	108.58

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	907	A	Sidechain
1	B	919	G	Sidechain
1	B	936	G	Sidechain
1	B	974	C	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	1555	0	792	96	0
2	A	4274	0	4165	165	0
3	A	32	0	22	2	0
4	A	36	0	0	0	0
4	B	18	0	0	2	0
All	All	5915	0	4979	249	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 23.

All (249) 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)
2:A:531:SER:HB3	2:A:537:VAL:H	1.28	0.98
1:B:933:U:H2'	1:B:935:U:OP1	1.66	0.94
2:A:529:ARG:HE	2:A:529:ARG:HA	1.36	0.88
1:B:954:U:O2'	1:B:955:U:H5'	1.78	0.83
2:A:39:LEU:HD13	2:A:81:ILE:HG12	1.62	0.81
2:A:341:ARG:HD3	2:A:369:PRO:HD2	1.63	0.81
2:A:343:MET:HE1	2:A:412:ARG:HB3	1.62	0.80
1:B:954:U:H2'	1:B:955:U:H6	1.45	0.79
1:B:963:U:H2'	1:B:964:C:C6	2.18	0.79
1:B:921:A:H61	1:B:947:A:H2'	1.49	0.78
2:A:403:LEU:HD13	2:A:409:VAL:HG22	1.67	0.76
1:B:908:U:H5'	1:B:949:C:OP2	1.86	0.75
2:A:412:ARG:HG2	2:A:412:ARG:HH11	1.51	0.75
1:B:943:G:O2'	1:B:944:C:H5'	1.86	0.75
2:A:362:MET:HG2	2:A:378:GLN:HG3	1.68	0.75
1:B:918:G:H4'	1:B:919:G:OP1	1.87	0.74
1:B:954:U:H2'	1:B:955:U:C6	2.23	0.73
1:B:919:G:O2'	1:B:920:U:C6	2.40	0.73
2:A:343:MET:HE3	2:A:458:TRP:H	1.53	0.73
1:B:950:G:O2'	1:B:951:A:H5'	1.91	0.71
2:A:463:HIS:O	2:A:505:PRO:HD3	1.91	0.71
1:B:907:A:H5'	1:B:908:U:OP2	1.92	0.70
1:B:958:A:HO2'	1:B:960:U:H5	1.40	0.70
2:A:362:MET:CG	2:A:378:GLN:HG3	2.21	0.70
1:B:939:U:H2'	1:B:940:C:O4'	1.93	0.68
2:A:289:ARG:HD3	2:A:495:SER:HB2	1.76	0.68
2:A:438:ASP:HB3	2:A:441:THR:OG1	1.94	0.68
1:B:958:A:O2'	1:B:960:U:H5	1.78	0.66
1:B:955:U:H2'	1:B:957:G:OP2	1.94	0.66
2:A:393:ARG:O	2:A:404:VAL:HA	1.96	0.65
2:A:412:ARG:HG2	2:A:412:ARG:NH1	2.09	0.64
1:B:918:G:H5''	1:B:919:G:OP1	1.97	0.64
2:A:471:LEU:HB2	2:A:497:VAL:HG13	1.79	0.64
1:B:930:G:O2'	1:B:931:A:H5'	1.98	0.64
1:B:952:G:H2'	1:B:953:G:O4'	1.97	0.64
2:A:410:ARG:HH21	2:A:442:LEU:HA	1.62	0.64
1:B:909:C:O2	1:B:945:A:N7	2.30	0.64
1:B:934:C:O2'	2:A:412:ARG:NH1	2.31	0.63
1:B:935:U:O4	2:A:341:ARG:NH1	2.31	0.63
2:A:346:ILE:HG13	2:A:469:ILE:HD12	1.81	0.63
1:B:956:C:H2'	1:B:957:G:O4'	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:909:C:C5'	1:B:910:G:OP2	2.47	0.62
1:B:903:G:O2'	1:B:904:G:H5'	1.99	0.62
1:B:909:C:C4	1:B:947:A:C2	2.87	0.62
1:B:939:U:C2	1:B:940:C:C6	2.87	0.62
2:A:28:HIS:HE1	2:A:62:ASN:OD1	1.83	0.62
1:B:918:G:O2'	1:B:957:G:N2	2.29	0.62
2:A:270:LYS:O	2:A:274:ASN:HB2	2.01	0.61
2:A:159:LYS:HD3	2:A:164:GLY:HA3	1.82	0.61
2:A:396:ALA:HB1	2:A:400:TYR:HB3	1.82	0.60
1:B:958:A:O2'	1:B:960:U:C5	2.51	0.60
2:A:159:LYS:HD2	2:A:165:PHE:CD2	2.36	0.60
2:A:349:VAL:HB	2:A:389:ARG:HG2	1.83	0.60
1:B:957:G:H2'	1:B:958:A:H5'	1.84	0.59
1:B:963:U:H2'	1:B:964:C:H6	1.64	0.59
1:B:918:G:C4'	1:B:919:G:OP1	2.50	0.59
1:B:908:U:H4'	1:B:948:G:H4'	1.85	0.59
2:A:529:ARG:HE	2:A:529:ARG:CA	2.14	0.59
1:B:909:C:H41	1:B:913:A:H2	1.45	0.58
2:A:433:ILE:HG22	2:A:435:CYS:SG	2.42	0.58
2:A:40:HIS:HA	2:A:292:THR:HA	1.85	0.58
2:A:114:ILE:HG21	2:A:154:LEU:HD13	1.83	0.58
2:A:416:VAL:HB	2:A:441:THR:HG21	1.86	0.58
1:B:916:C:H5'	1:B:960:U:O2	2.03	0.58
1:B:916:C:OP2	1:B:916:C:H3'	2.03	0.58
2:A:478:VAL:O	2:A:481:PRO:HD3	2.03	0.58
1:B:948:G:O2'	1:B:949:C:P	2.62	0.57
2:A:32:PRO:HA	2:A:64:ARG:O	2.04	0.57
1:B:941:C:C2	1:B:942:G:C8	2.92	0.57
2:A:531:SER:HB3	2:A:537:VAL:N	2.10	0.57
2:A:424:LYS:HD3	2:A:428:GLY:O	2.05	0.57
1:B:921:A:H61	1:B:947:A:C2'	2.14	0.57
2:A:126:PRO:O	2:A:129:ILE:HG22	2.05	0.57
2:A:528:SER:O	2:A:529:ARG:NE	2.37	0.57
2:A:410:ARG:NH2	2:A:442:LEU:HA	2.20	0.57
2:A:343:MET:HE1	2:A:412:ARG:CB	2.35	0.56
2:A:419:ALA:HA	2:A:435:CYS:SG	2.46	0.56
2:A:512:ALA:HB1	2:A:528:SER:HB2	1.86	0.56
1:B:914:A:C6	1:B:915:G:C2	2.94	0.56
2:A:30:ARG:NH1	2:A:215:HIS:NE2	2.53	0.55
2:A:166:GLU:O	2:A:169:LYS:HB2	2.06	0.55
1:B:975:C:H2'	1:B:976:A:O4'	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:240:TYR:OH	2:A:253:PRO:HB2	2.08	0.54
2:A:363:VAL:HG22	2:A:379:VAL:O	2.07	0.54
1:B:960:U:H5'	1:B:961:C:OP2	2.08	0.53
2:A:331:ILE:HG13	2:A:335:LEU:HD22	1.89	0.53
2:A:149:SER:OG	2:A:152:GLU:HG3	2.08	0.53
1:B:902:G:C8	2:A:137:THR:HG22	2.43	0.53
2:A:30:ARG:NH2	2:A:228:LEU:O	2.42	0.53
2:A:410:ARG:HD3	2:A:416:VAL:HG22	1.91	0.53
1:B:955:U:C2'	1:B:957:G:OP2	2.57	0.52
2:A:152:GLU:O	2:A:156:LEU:HD22	2.09	0.52
2:A:529:ARG:HA	2:A:529:ARG:NE	2.17	0.52
1:B:947:A:O2'	1:B:948:G:H5'	2.10	0.52
2:A:282:VAL:HG12	2:A:289:ARG:NH1	2.26	0.51
2:A:136:LEU:HD23	2:A:183:ILE:HD11	1.92	0.51
2:A:322:ILE:HD12	2:A:322:ILE:N	2.26	0.51
2:A:512:ALA:HB1	2:A:528:SER:CB	2.40	0.51
2:A:324:MET:O	2:A:328:GLU:HG3	2.11	0.51
2:A:132:TYR:CD2	2:A:141:LYS:HG3	2.45	0.51
1:B:944:C:H2'	1:B:945:A:C4	2.46	0.51
2:A:180:SER:O	2:A:186:ARG:NH1	2.43	0.51
2:A:397:ASN:HD21	2:A:399:GLN:HB2	1.76	0.51
1:B:921:A:N1	1:B:947:A:C4	2.78	0.50
1:B:918:G:C5'	1:B:919:G:OP1	2.60	0.50
1:B:939:U:C4	1:B:940:C:C5	2.99	0.50
1:B:926:A:H2'	1:B:927:C:O4'	2.11	0.50
2:A:301:TYR:CE2	2:A:327:LEU:HD22	2.47	0.50
2:A:80:SER:O	2:A:83:ASN:HB3	2.12	0.50
2:A:534:GLU:O	2:A:536:PRO:HD3	2.12	0.50
2:A:343:MET:CE	2:A:412:ARG:HB3	2.36	0.50
1:B:943:G:C2'	1:B:944:C:H5'	2.42	0.50
2:A:46:SER:HB2	3:A:998:QSI:H1'	1.94	0.49
2:A:282:VAL:HG12	2:A:289:ARG:HH11	1.76	0.49
2:A:472:TYR:HA	2:A:495:SER:O	2.12	0.49
2:A:192:ARG:HD3	2:A:194:LYS:HE3	1.93	0.49
2:A:129:ILE:HG13	2:A:173:ARG:NH2	2.28	0.49
2:A:391:ASP:HA	2:A:402:ARG:HD2	1.95	0.49
2:A:500:GLN:OE1	2:A:500:GLN:HA	2.12	0.49
1:B:909:C:N3	1:B:947:A:C2	2.80	0.49
2:A:288:PRO:HG3	2:A:298:ARG:HG2	1.94	0.49
2:A:229:CYS:O	2:A:257:GLU:HA	2.12	0.48
1:B:902:G:H5''	4:B:48:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:974:C:N3	2:A:168:GLY:HA2	2.28	0.48
1:B:914:A:N6	1:B:915:G:C2	2.82	0.48
1:B:903:G:HO2'	1:B:904:G:H5'	1.79	0.48
2:A:176:ILE:HG21	2:A:185:MET:HE3	1.96	0.48
1:B:921:A:C2	1:B:947:A:C2	3.02	0.48
2:A:260:ARG:HB2	3:A:998:QSI:C6	2.44	0.48
2:A:385:ILE:HA	2:A:460:SER:HA	1.95	0.48
1:B:902:G:C5'	4:B:48:HOH:O	2.62	0.47
1:B:909:C:H5'	1:B:910:G:OP2	2.14	0.47
2:A:397:ASN:ND2	2:A:399:GLN:HB2	2.28	0.47
2:A:341:ARG:HD3	2:A:369:PRO:CD	2.37	0.47
2:A:343:MET:HE1	2:A:457:HIS:HA	1.97	0.47
2:A:347:ASP:O	2:A:388:ASP:HA	2.13	0.47
2:A:377:ARG:HG2	2:A:377:ARG:HH11	1.79	0.47
2:A:422:VAL:HG23	2:A:433:ILE:HG13	1.96	0.47
2:A:522:GLY:HA2	2:A:544:LEU:CD1	2.44	0.47
1:B:954:U:H2'	1:B:955:U:O4'	2.15	0.46
2:A:110:ALA:O	2:A:114:ILE:HG13	2.15	0.46
2:A:227:SER:O	2:A:255:GLN:HA	2.14	0.46
2:A:393:ARG:HG2	2:A:395:GLU:O	2.15	0.46
1:B:934:C:HO2'	2:A:412:ARG:NH1	2.12	0.46
2:A:150:VAL:HG12	2:A:154:LEU:HD22	1.95	0.46
2:A:71:VAL:HG23	2:A:72:LYS:NZ	2.31	0.46
1:B:974:C:H1'	2:A:192:ARG:HB3	1.97	0.46
1:B:936:G:C6	2:A:401:LYS:HG2	2.50	0.46
2:A:236:ASN:H	2:A:236:ASN:HD22	1.62	0.46
2:A:422:VAL:HG21	2:A:430:ILE:HD13	1.98	0.46
1:B:952:G:C4	1:B:953:G:C8	3.03	0.46
2:A:231:LEU:HD22	2:A:259:SER:HA	1.98	0.46
1:B:921:A:N6	1:B:947:A:H2'	2.25	0.46
2:A:335:LEU:HB3	2:A:523:TYR:CD1	2.51	0.46
2:A:157:PHE:O	2:A:160:MET:HB2	2.16	0.46
2:A:82:LYS:O	2:A:86:GLU:HG3	2.15	0.45
2:A:377:ARG:HG2	2:A:377:ARG:NH1	2.30	0.45
1:B:935:U:C5	1:B:937:A:C2	3.04	0.45
2:A:136:LEU:HD23	2:A:183:ILE:CD1	2.47	0.45
1:B:919:G:C4	1:B:957:G:N2	2.84	0.45
1:B:954:U:C2'	1:B:955:U:H5'	2.46	0.45
2:A:238:ARG:HD2	2:A:238:ARG:N	2.32	0.45
1:B:934:C:N4	2:A:410:ARG:HH21	2.14	0.45
2:A:346:ILE:HG13	2:A:469:ILE:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:351:LEU:C	2:A:351:LEU:HD23	2.41	0.45
2:A:386:TRP:N	2:A:459:VAL:O	2.49	0.45
2:A:43:HIS:CE1	2:A:270:LYS:HE3	2.51	0.45
2:A:397:ASN:ND2	2:A:399:GLN:H	2.15	0.45
2:A:192:ARG:NE	2:A:194:LYS:HE3	2.32	0.45
1:B:916:C:C5'	1:B:960:U:O2	2.63	0.44
2:A:230:THR:HG21	2:A:260:ARG:HB3	1.99	0.44
1:B:959:A:C6	1:B:960:U:C2	3.06	0.44
2:A:393:ARG:HB2	2:A:400:TYR:CZ	2.53	0.44
2:A:522:GLY:HA2	2:A:544:LEU:HD13	1.97	0.44
1:B:907:A:C5'	1:B:908:U:OP2	2.61	0.44
2:A:340:PRO:HA	2:A:367:ASN:O	2.15	0.44
2:A:44:ALA:HB2	2:A:293:ILE:HD11	2.00	0.44
1:B:963:U:O2'	1:B:964:C:H5'	2.18	0.44
2:A:43:HIS:HE1	2:A:270:LYS:HE3	1.82	0.44
2:A:411:LEU:HA	2:A:411:LEU:HD23	1.82	0.44
2:A:184:VAL:HG22	2:A:239:LEU:HD22	1.99	0.44
1:B:909:C:H5''	1:B:910:G:OP2	2.18	0.44
2:A:114:ILE:CG2	2:A:154:LEU:HD13	2.47	0.44
1:B:914:A:N6	1:B:915:G:N1	2.66	0.44
2:A:286:ASP:O	2:A:298:ARG:HD3	2.18	0.44
2:A:268:MET:HE2	2:A:268:MET:HB2	1.89	0.43
2:A:38:TYR:HB2	2:A:285:TRP:CE3	2.53	0.43
2:A:159:LYS:HD2	2:A:165:PHE:CE2	2.52	0.43
2:A:341:ARG:H	2:A:341:ARG:HD2	1.84	0.43
1:B:907:A:C4'	1:B:908:U:OP2	2.66	0.43
1:B:929:G:C6	1:B:942:G:C6	3.06	0.43
1:B:934:C:O2'	2:A:412:ARG:NH2	2.51	0.43
1:B:968:C:H2'	1:B:969:C:H6	1.83	0.43
1:B:903:G:C2'	1:B:904:G:H5'	2.49	0.43
2:A:183:ILE:HA	2:A:186:ARG:HG3	1.99	0.43
2:A:11:ILE:HD13	2:A:228:LEU:HD22	2.00	0.43
1:B:937:A:H2'	1:B:938:U:C5'	2.48	0.43
1:B:939:U:C2'	1:B:940:C:H5'	2.49	0.43
1:B:976:A:C2	2:A:233:PHE:CZ	3.07	0.43
1:B:952:G:C6	1:B:953:G:C5	3.07	0.43
2:A:32:PRO:HG3	2:A:215:HIS:HE1	1.84	0.43
2:A:192:ARG:HE	2:A:194:LYS:HE3	1.83	0.43
2:A:263:LEU:HB2	2:A:268:MET:HE1	2.00	0.43
2:A:403:LEU:HD21	2:A:419:ALA:HB2	2.00	0.43
2:A:173:ARG:HD2	2:A:187:ASP:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:524:PHE:HA	2:A:539:ASN:O	2.19	0.43
1:B:938:U:H4'	2:A:336:ASN:OD1	2.19	0.42
2:A:438:ASP:CG	2:A:441:THR:HG23	2.44	0.42
2:A:41:ILE:HG22	2:A:268:MET:SD	2.59	0.42
2:A:51:PHE:O	2:A:55:GLN:HG2	2.19	0.42
1:B:929:G:C2	1:B:942:G:C4	3.07	0.42
2:A:505:PRO:O	2:A:508:LYS:HB3	2.20	0.42
1:B:909:C:H5	1:B:912:C:H41	1.67	0.42
1:B:937:A:C2'	1:B:938:U:H5'	2.49	0.42
1:B:954:U:C2	1:B:955:U:C6	3.08	0.42
1:B:964:C:H2'	1:B:965:G:O4'	2.20	0.42
2:A:43:HIS:O	2:A:47:ILE:HG13	2.20	0.42
1:B:948:G:HO2'	1:B:949:C:P	2.43	0.42
2:A:340:PRO:CD	2:A:514:LYS:HE3	2.50	0.42
2:A:341:ARG:HD2	2:A:341:ARG:N	2.35	0.42
1:B:968:C:H2'	1:B:969:C:C6	2.55	0.42
2:A:121:VAL:H	2:A:153:ASN:ND2	2.18	0.42
2:A:362:MET:HG2	2:A:378:GLN:CG	2.45	0.42
2:A:427:GLU:O	2:A:427:GLU:HG2	2.19	0.42
2:A:524:PHE:CE2	2:A:540:ARG:HB2	2.55	0.41
1:B:966:U:O2'	1:B:967:A:H5'	2.20	0.41
2:A:353:ILE:HG21	2:A:437:TYR:HB3	2.02	0.41
2:A:407:LYS:HG3	2:A:408:GLU:N	2.35	0.41
2:A:464:ALA:O	2:A:466:PRO:HD3	2.21	0.41
1:B:934:C:O2'	2:A:412:ARG:CZ	2.69	0.41
2:A:64:ARG:HA	2:A:97:ARG:O	2.20	0.41
2:A:50:ASN:OD1	2:A:228:LEU:HD12	2.21	0.41
2:A:236:ASN:HD22	2:A:236:ASN:N	2.18	0.41
1:B:967:A:H2'	1:B:968:C:C6	2.56	0.41
2:A:231:LEU:O	2:A:234:GLN:HG3	2.21	0.41
2:A:254:ARG:HA	2:A:254:ARG:HD3	1.86	0.41
2:A:457:HIS:HD2	2:A:520:ARG:HE	1.69	0.41
2:A:512:ALA:N	2:A:526:LEU:HD23	2.35	0.41
2:A:53:ILE:O	2:A:57:TYR:HD1	2.05	0.41
2:A:75:ILE:O	2:A:79:GLU:HG3	2.21	0.41
2:A:368:HIS:HB2	2:A:374:MET:SD	2.61	0.41
2:A:45:LYS:HD2	2:A:261:LEU:HB2	2.02	0.40
2:A:41:ILE:CG2	2:A:268:MET:SD	3.09	0.40
2:A:60:GLN:HB3	2:A:93:SER:HB2	2.04	0.40
2:A:425:ASP:OD1	2:A:429:ASN:HB2	2.22	0.40
2:A:166:GLU:HB2	2:A:169:LYS:HD3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:225:THR:OG1	2:A:226:HIS:HD2	2.04	0.40
1:B:939:U:C4	1:B:940:C:C4	3.09	0.40
2:A:402:ARG:HD3	2:A:520:ARG:HH22	1.85	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%)	488 (93%)	30 (6%)	7 (1%)	9	21

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	32	PRO
2	A	405	LEU
2	A	527	ASP
2	A	531	SER
2	A	426	ALA
2	A	348	PRO
2	A	176	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	462/478 (97%)	419 (91%)	43 (9%)	8 18

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

Mol	Chain	Res	Type
2	A	19	LEU
2	A	27	VAL
2	A	30	ARG
2	A	32	PRO
2	A	39	LEU
2	A	49	LEU
2	A	66	ASP
2	A	78	VAL
2	A	105	GLN
2	A	106	LEU
2	A	124	LEU
2	A	126	PRO
2	A	154	LEU
2	A	156	LEU
2	A	159	LYS
2	A	173	ARG
2	A	180	SER
2	A	186	ARG
2	A	190	LEU
2	A	192	ARG
2	A	231	LEU
2	A	236	ASN
2	A	263	LEU
2	A	266	THR
2	A	327	LEU
2	A	335	LEU
2	A	341	ARG
2	A	352	VAL
2	A	365	MET
2	A	369	PRO
2	A	395	GLU
2	A	408	GLU
2	A	412	ARG
2	A	432	THR
2	A	441	THR
2	A	442	LEU
2	A	463	HIS
2	A	467	VAL

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Mol	Chain	Res	Type
2	A	475	LEU
2	A	497	VAL
2	A	507	LEU
2	A	511	VAL
2	A	529	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	28	HIS
2	A	115	ASN
2	A	142	ASN
2	A	153	ASN
2	A	226	HIS
2	A	236	ASN
2	A	397	ASN
2	A	413	ASN
2	A	429	ASN
2	A	457	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	72/74 (97%)	20 (27%)	11 (15%)

All (20) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	907	A
1	B	908	U
1	B	909	C
1	B	910	G
1	B	916	C
1	B	918	G
1	B	919	G
1	B	920	U
1	B	921	A
1	B	934	C
1	B	935	U
1	B	936	G

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Mol	Chain	Res	Type
1	B	937	A
1	B	941	C
1	B	949	C
1	B	956	C
1	B	961	C
1	B	965	G
1	B	973	G
1	B	974	C

All (11) 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	934	C
1	B	935	U
1	B	936	G
1	B	948	G
1	B	960	U
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 oligosaccharides 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	-	34,34,34	2.21	6 (17%)	47,50,50	0.65	1 (2%)

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	QSI	A	998	-	-	4/23/40/40	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	9.02	1.50	1.42
3	A	998	QSI	S-N10	5.23	1.68	1.59
3	A	998	QSI	CD-NE2	4.37	1.46	1.32
3	A	998	QSI	O5'-S	-4.28	1.51	1.60
3	A	998	QSI	C-N10	2.95	1.42	1.37
3	A	998	QSI	CA-N	-2.94	1.33	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	998	QSI	C5'-O5'-S	2.28	121.75	116.97

There are no chirality outliers.

All (4) torsion outliers are listed below:

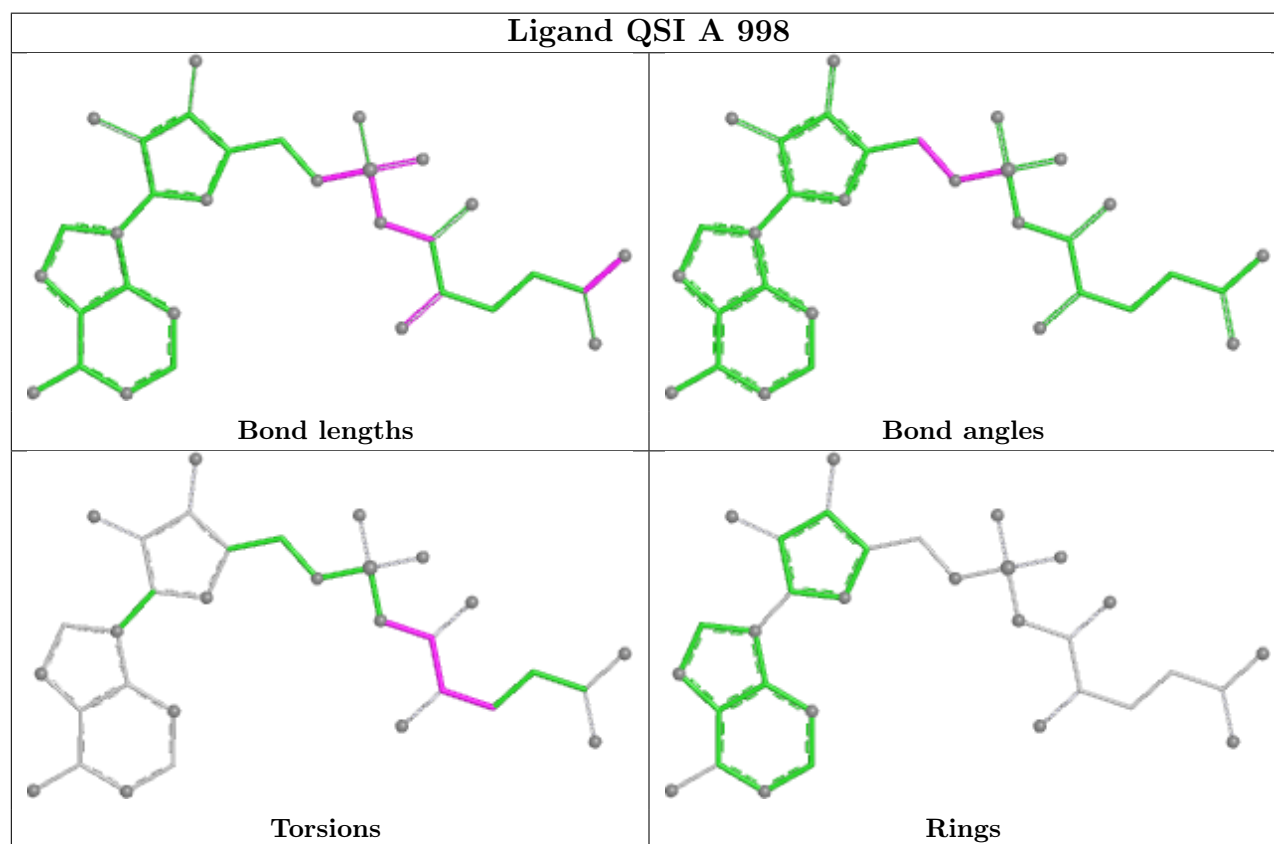
Mol	Chain	Res	Type	Atoms
3	A	998	QSI	N-CA-CB-CG
3	A	998	QSI	C-CA-CB-CG
3	A	998	QSI	O-C-N10-S
3	A	998	QSI	N10-C-CA-N

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	998	QSI	2	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 ⓘ

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	B	73/74 (98%)	2.87	35 (47%) 0 0	0, 55, 85, 87	0
2	A	529/548 (96%)	0.69	61 (11%) 9 7	6, 28, 67, 94	0
All	All	602/622 (96%)	0.96	96 (15%) 5 4	0, 30, 75, 94	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	953	G	12.2
1	B	916	C	10.5
1	B	920	U	9.3
1	B	945	A	9.2
1	B	963	U	8.4
1	B	955	U	8.3
1	B	954	U	8.1
1	B	952	G	7.7
2	A	440	ASP	7.6
2	A	529	ARG	7.3
2	A	397	ASN	6.9
1	B	942	G	6.4
2	A	441	THR	6.0
1	B	956	C	5.9
1	B	947	A	5.9
1	B	919	G	5.9
1	B	958	A	5.8
1	B	918	G	5.8
1	B	909	C	5.7
1	B	957	G	5.7
2	A	406	GLY	5.5
2	A	547	THR	5.2
1	B	951	A	5.1
2	A	396	ALA	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	921	A	5.1
2	A	528	SER	5.0
2	A	442	LEU	4.9
2	A	512	ALA	4.7
1	B	943	G	4.5
2	A	393	ARG	4.5
2	A	531	SER	4.5
2	A	439	ALA	4.5
2	A	454	GLY	4.5
1	B	964	C	4.5
2	A	398	LYS	4.5
1	B	941	C	4.4
1	B	962	C	4.4
2	A	419	ALA	4.4
2	A	408	GLU	4.2
2	A	534	GLU	4.2
1	B	915	G	4.2
1	B	965	G	4.0
2	A	404	VAL	4.0
2	A	399	GLN	3.8
2	A	414	ALA	3.7
2	A	532	THR	3.6
2	A	353	ILE	3.6
2	A	415	TYR	3.6
2	A	426	ALA	3.6
2	A	347	ASP	3.5
2	A	357	GLN	3.5
1	B	944	C	3.4
2	A	527	ASP	3.3
2	A	405	LEU	3.2
2	A	431	THR	3.1
2	A	374	MET	3.1
2	A	421	ARG	3.1
2	A	376	SER	3.1
2	A	354	GLU	3.0
2	A	72	LYS	2.9
2	A	25	THR	2.9
1	B	931	A	2.8
1	B	948	G	2.7
2	A	400	TYR	2.6
2	A	409	VAL	2.6
1	B	929	G	2.5

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Mol	Chain	Res	Type	RSRZ
2	A	427	GLU	2.5
2	A	336	ASN	2.5
1	B	922	A	2.5
2	A	355	ASN	2.4
2	A	455	VAL	2.4
2	A	511	VAL	2.4
2	A	457	HIS	2.4
2	A	423	GLU	2.4
2	A	138	GLN	2.4
2	A	363	VAL	2.4
2	A	407	LYS	2.3
2	A	403	LEU	2.3
2	A	483	ALA	2.3
2	A	526	LEU	2.3
1	B	928	C	2.3
1	B	959	A	2.2
2	A	392	PHE	2.2
2	A	368	HIS	2.2
1	B	935	U	2.2
2	A	395	GLU	2.2
2	A	536	PRO	2.2
2	A	204	LYS	2.2
2	A	318	GLN	2.1
1	B	932	U	2.1
1	B	933	U	2.1
2	A	422	VAL	2.1
1	B	961	C	2.1
2	A	545	ARG	2.1
2	A	413	ASN	2.0
2	A	271	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

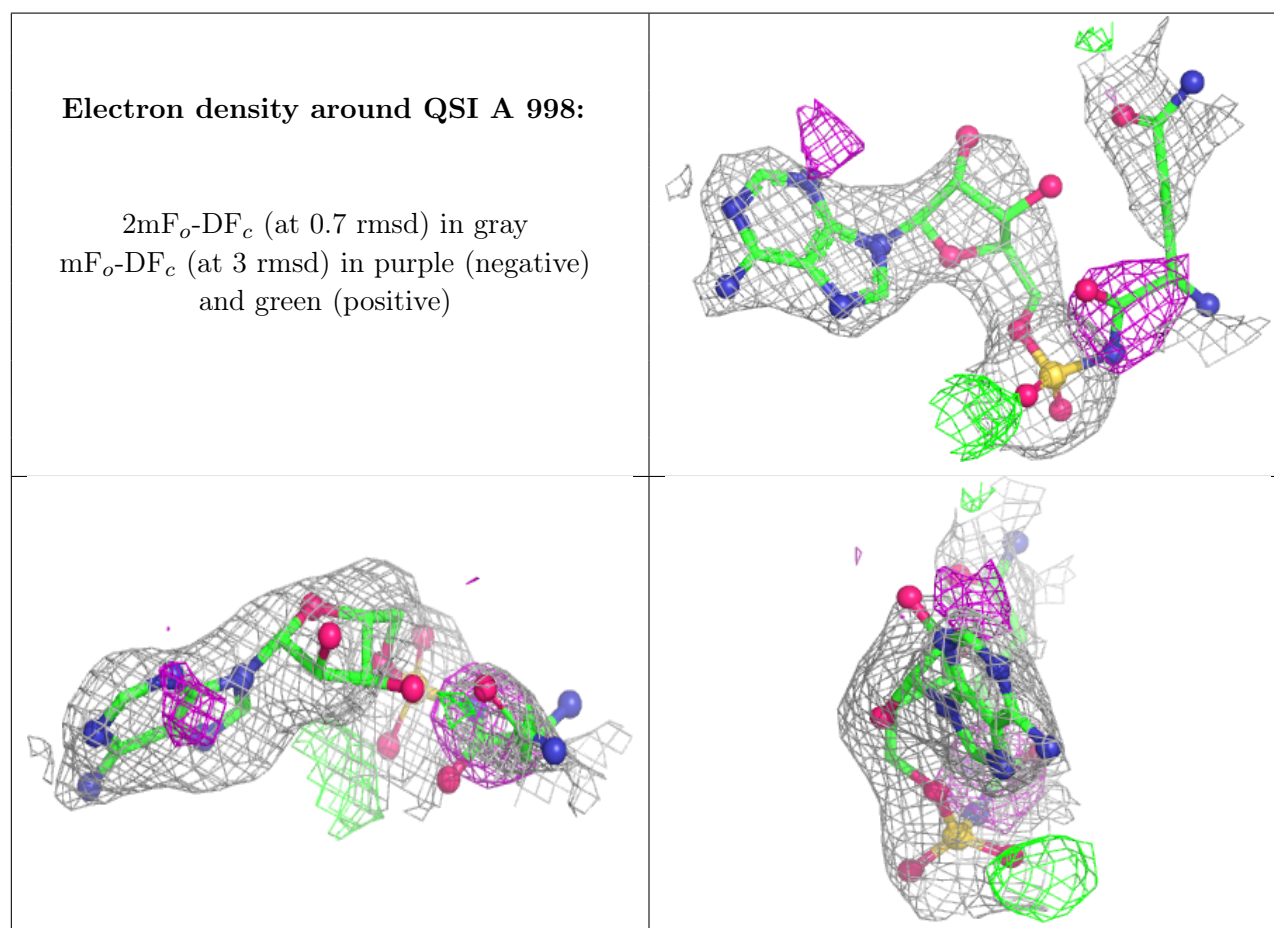
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	QSI	A	998	32/32	0.83	0.16	25,44,56,59	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.