Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2021 – 07:01 AM EDT

PDB ID	:	2RD2
Title	:	Glutaminyl-tRNA synthetase mutant C229R with bound analog 5'-O-[N-(L-GLUTAMINYL)-SULFAMOYL]ADENOSINE
Authors	:	Bullock, T.L.; Perona, J.J.
Deposited on	:	2007-09-20
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

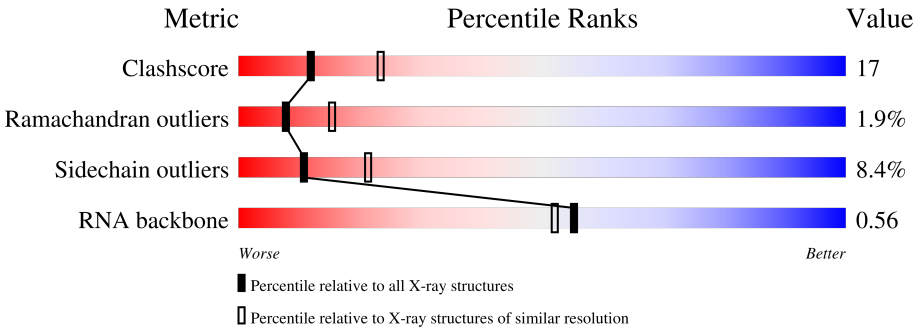
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	75	40% 39% 17% • •
2	A	556	63% 27% 5% 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6032 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 Glutamine tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	B	74	1570	702	279	516	73	0	0	0

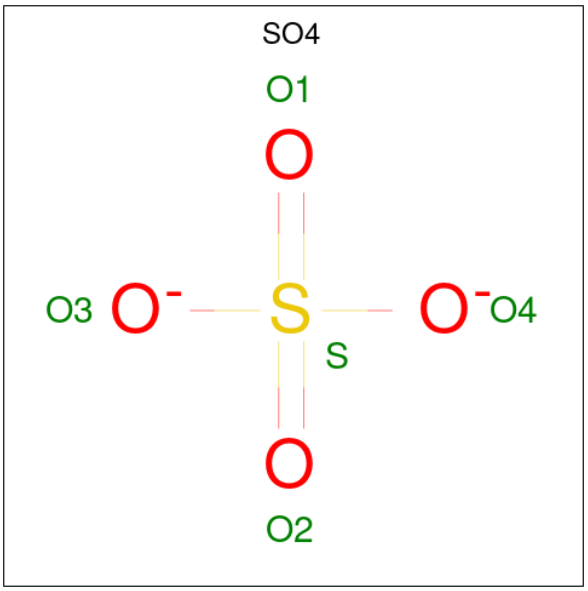
- Molecule 2 is a protein called Glutaminyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	529	4284	2707	755	802	20	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

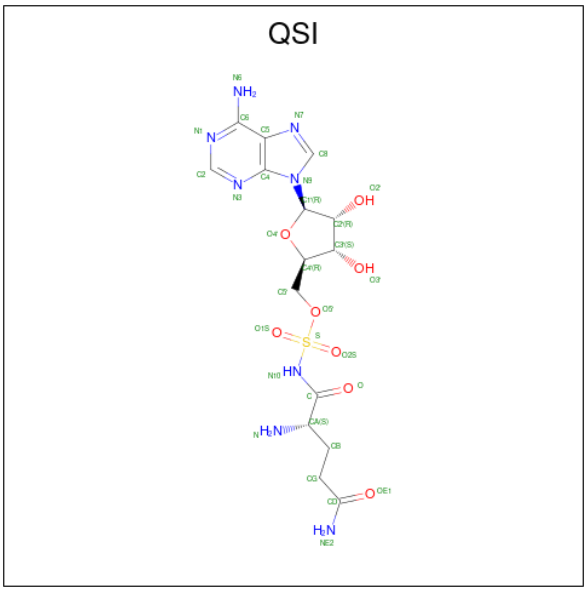
Chain	Residue	Modelled	Actual	Comment	Reference
A	229	ARG	CYS	engineered mutation	UNP P00962
A	548	LEU	-	expression tag	UNP P00962
A	549	GLU	-	expression tag	UNP P00962
A	550	HIS	-	expression tag	UNP P00962
A	551	HIS	-	expression tag	UNP P00962
A	552	HIS	-	expression tag	UNP P00962
A	553	HIS	-	expression tag	UNP P00962
A	554	HIS	-	expression tag	UNP P00962
A	555	HIS	-	expression tag	UNP P00962

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is 5'-O-[N-(L-GLUTAMINYL)-SULFAMOYL]ADENOSINE (three-letter code: QSI) (formula: $C_{15}H_{22}N_8O_8S$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	B	26	26	26	0	0
			Total	O		
5	A	110	110	110	0	0

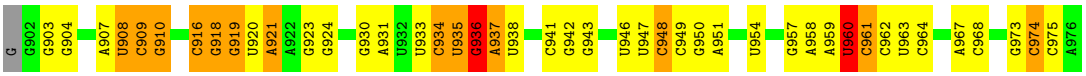
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

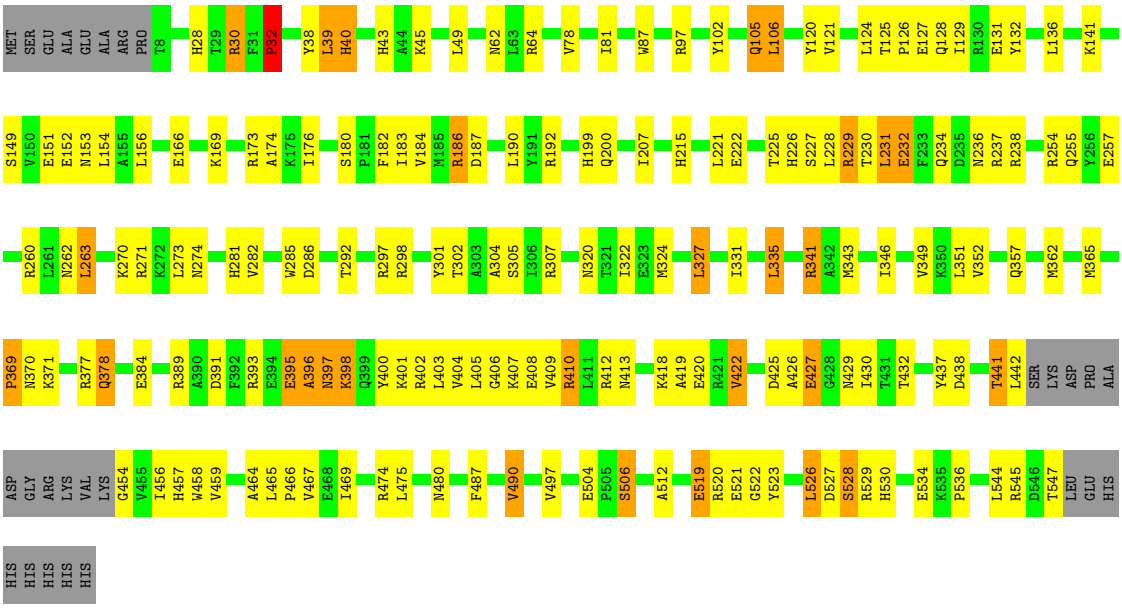
- Molecule 1: Glutamine tRNA

Chain B: 40% 39% 17%



- Molecule 2: Glutaminyl-tRNA synthetase

Chain A: 63% 27% 5% 5%



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	237.66Å 93.34Å 114.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	119.50 – 2.60	Depositor
% Data completeness (in resolution range)	94.0 (119.50-2.60)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.209 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6032	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

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: SO4, 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	0.35	0/1753	0.77	2/2730 (0.1%)
2	A	0.40	0/4384	0.62	0/5934
All	All	0.39	0/6137	0.67	2/8664 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	974	C	N1-C1'-C2'	6.16	122.01	114.00
1	B	936	G	N9-C1'-C2'	5.85	121.60	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	960	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	1570	0	801	43	0
2	A	4284	0	4180	151	0
3	A	10	0	0	0	0
4	A	32	0	22	3	0
5	A	110	0	0	13	0
5	B	26	0	0	0	0
All	All	6032	0	5003	188	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 17.

All (188) 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:526:LEU:HG	2:A:527:ASP:H	1.31	0.93
1:B:950:G:H1	1:B:964:C:H42	1.23	0.87
2:A:136:LEU:HD23	2:A:183:ILE:HD11	1.58	0.83
2:A:352:VAL:HG12	2:A:384:GLU:HG2	1.63	0.80
2:A:39:LEU:HD13	2:A:81:ILE:HG12	1.64	0.79
2:A:362:MET:HG2	2:A:378:GLN:HG3	1.65	0.78
1:B:935:U:O2'	2:A:520:ARG:HG2	1.85	0.76
2:A:341:ARG:HB3	5:A:1487:HOH:O	1.84	0.76
2:A:403:LEU:HD13	2:A:409:VAL:HG22	1.69	0.74
2:A:522:GLY:HA2	2:A:544:LEU:HD13	1.70	0.73
2:A:237:ARG:HA	2:A:255:GLN:HE22	1.56	0.71
2:A:304:ALA:HA	2:A:307:ARG:NH1	2.06	0.71
1:B:918:G:H5"	1:B:919:G:OP1	1.90	0.70
2:A:362:MET:CG	2:A:378:GLN:HG3	2.22	0.69
1:B:935:U:O4	2:A:341:ARG:NH1	2.25	0.69
1:B:954:U:H3	1:B:958:A:H62	1.40	0.68
2:A:519:GLU:HB2	5:A:1487:HOH:O	1.92	0.67
1:B:930:G:O2'	1:B:931:A:H5'	1.95	0.65
2:A:125:THR:OG1	2:A:128:GLN:HG3	1.96	0.65
2:A:343:MET:HE3	2:A:458:TRP:H	1.61	0.64
2:A:127:GLU:O	2:A:131:GLU:HG3	1.98	0.63
1:B:903:G:O2'	1:B:904:G:H5'	1.98	0.63
2:A:40:HIS:HA	2:A:292:THR:HA	1.81	0.63
2:A:343:MET:HE1	2:A:457:HIS:HA	1.81	0.62
2:A:121:VAL:H	2:A:153:ASN:ND2	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:230:THR:HB	2:A:232:GLU:OE1	1.99	0.61
2:A:273:LEU:HD12	5:A:1505:HOH:O	1.98	0.61
2:A:102:TYR:O	2:A:106:LEU:HD22	2.01	0.61
1:B:950:G:H1	1:B:964:C:N4	1.95	0.60
1:B:960:U:H5'	1:B:961:C:OP2	2.01	0.60
1:B:934:C:H5"	1:B:935:U:OP1	2.02	0.60
2:A:151:GLU:H	2:A:151:GLU:CD	2.04	0.60
2:A:173:ARG:HD2	2:A:187:ASP:O	2.01	0.60
2:A:357:GLN:H	2:A:357:GLN:CD	2.05	0.59
2:A:391:ASP:HA	2:A:402:ARG:HD2	1.84	0.59
2:A:301:TYR:CE2	2:A:327:LEU:HD22	2.37	0.59
2:A:529:ARG:HA	2:A:529:ARG:HE	1.68	0.59
2:A:263:LEU:HD13	2:A:324:MET:HE2	1.85	0.59
1:B:963:U:H2'	1:B:964:C:C6	2.38	0.59
2:A:263:LEU:HD13	2:A:324:MET:CE	2.32	0.59
1:B:909:C:H4'	1:B:910:G:OP1	2.02	0.58
1:B:961:C:H2'	1:B:962:C:H6	1.69	0.58
2:A:125:THR:HG23	2:A:128:GLN:HE21	1.68	0.58
2:A:346:ILE:HG12	2:A:469:ILE:HD13	1.85	0.58
1:B:918:G:O2'	1:B:957:G:N2	2.37	0.58
2:A:271:ARG:HD3	2:A:271:ARG:C	2.25	0.57
1:B:934:C:N4	2:A:410:ARG:HH21	2.03	0.57
2:A:126:PRO:O	2:A:129:ILE:HG22	2.04	0.57
2:A:395:GLU:H	2:A:395:GLU:CD	2.08	0.57
2:A:526:LEU:HG	2:A:527:ASP:N	2.13	0.56
1:B:958:A:HO2'	1:B:960:U:H5	1.53	0.56
2:A:398:LYS:H	2:A:398:LYS:HD2	1.71	0.56
2:A:442:LEU:HD23	2:A:442:LEU:N	2.21	0.55
2:A:331:ILE:HG13	2:A:335:LEU:HD22	1.89	0.55
2:A:30:ARG:NH2	2:A:228:LEU:O	2.40	0.55
2:A:166:GLU:O	2:A:169:LYS:HB2	2.07	0.55
2:A:480:ASN:HA	5:A:1456:HOH:O	2.08	0.54
2:A:132:TYR:CD2	2:A:141:LYS:HG3	2.42	0.54
2:A:301:TYR:HE2	2:A:327:LEU:HD22	1.73	0.54
2:A:400:TYR:CZ	2:A:402:ARG:HB2	2.42	0.53
2:A:534:GLU:O	2:A:536:PRO:HD3	2.08	0.53
2:A:401:LYS:O	2:A:454:GLY:HA3	2.08	0.53
2:A:410:ARG:HH21	2:A:442:LEU:HA	1.74	0.53
2:A:377:ARG:HH11	2:A:377:ARG:HG2	1.75	0.52
2:A:410:ARG:NH2	2:A:442:LEU:HA	2.23	0.52
1:B:963:U:H2'	1:B:964:C:H6	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:346:ILE:HG12	2:A:469:ILE:CD1	2.40	0.52
2:A:395:GLU:OE2	2:A:396:ALA:N	2.43	0.52
1:B:967:A:H2'	1:B:968:C:C6	2.45	0.52
2:A:271:ARG:HD3	2:A:271:ARG:O	2.10	0.52
1:B:918:G:H2'	1:B:957:G:H22	1.73	0.52
1:B:908:U:O4'	1:B:948:C:O2'	2.28	0.52
2:A:64:ARG:HA	2:A:97:ARG:O	2.10	0.52
2:A:286:ASP:O	2:A:298:ARG:HD3	2.10	0.51
2:A:229:ARG:HB3	4:A:998:QSI:HN22	1.75	0.51
2:A:465:LEU:HD12	2:A:466:PRO:HD2	1.93	0.51
1:B:937:A:H2'	1:B:938:U:O4'	2.11	0.51
2:A:40:HIS:HD2	5:A:1505:HOH:O	1.92	0.51
2:A:341:ARG:N	2:A:341:ARG:HD2	2.25	0.51
2:A:335:LEU:HB3	2:A:523:TYR:CD1	2.46	0.51
2:A:504:GLU:OE2	2:A:506:SER:HB3	2.11	0.51
2:A:39:LEU:CD1	2:A:81:ILE:HG12	2.38	0.51
2:A:398:LYS:HD2	2:A:398:LYS:N	2.25	0.51
2:A:504:GLU:HG3	2:A:506:SER:HB3	1.93	0.50
2:A:151:GLU:CD	2:A:151:GLU:N	2.65	0.50
2:A:391:ASP:OD1	2:A:402:ARG:HD3	2.11	0.50
1:B:933:U:H2'	1:B:935:U:OP1	2.12	0.50
2:A:149:SER:OG	2:A:152:GLU:HG3	2.12	0.49
2:A:236:ASN:H	2:A:236:ASN:HD22	1.60	0.49
4:A:998:QSI:H3'	4:A:998:QSI:HB1	1.93	0.49
2:A:262:ASN:HB2	2:A:320:ASN:O	2.12	0.49
2:A:419:ALA:O	2:A:420:GLU:HG3	2.12	0.49
1:B:962:C:O2'	1:B:963:U:H5'	2.12	0.49
2:A:40:HIS:CD2	5:A:1505:HOH:O	2.66	0.48
2:A:425:ASP:OD1	2:A:429:ASN:HB2	2.13	0.48
2:A:229:ARG:NE	5:A:1464:HOH:O	2.36	0.48
2:A:527:ASP:CG	2:A:529:ARG:H	2.16	0.48
2:A:438:ASP:CG	2:A:441:THR:HG23	2.34	0.48
2:A:487:PHE:O	2:A:490:VAL:HG12	2.13	0.48
2:A:121:VAL:H	2:A:153:ASN:HD22	1.61	0.47
2:A:357:GLN:CD	2:A:357:GLN:N	2.68	0.47
2:A:534:GLU:H	2:A:534:GLU:CD	2.18	0.47
1:B:958:A:O2'	1:B:960:U:H5	1.97	0.47
2:A:120:TYR:HB2	2:A:153:ASN:HD21	1.79	0.47
2:A:254:ARG:HD2	5:A:1489:HOH:O	2.14	0.47
1:B:958:A:O2'	1:B:960:U:C5	2.66	0.47
1:B:942:G:O2'	1:B:943:G:H5'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:28:HIS:HE1	2:A:62:ASN:OD1	1.97	0.47
2:A:351:LEU:HD23	2:A:351:LEU:O	2.14	0.47
2:A:64:ARG:HD3	2:A:222:GLU:OE2	2.15	0.46
2:A:180:SER:O	2:A:186:ARG:NH1	2.48	0.46
2:A:38:TYR:HB2	2:A:285:TRP:CE3	2.50	0.46
2:A:407:LYS:HG3	2:A:408:GLU:N	2.29	0.46
2:A:459:VAL:HG12	2:A:464:ALA:HB2	1.98	0.46
2:A:528:SER:C	2:A:530:HIS:H	2.19	0.46
2:A:32:PRO:HA	2:A:64:ARG:O	2.15	0.46
2:A:393:ARG:HB3	2:A:396:ALA:HB2	1.98	0.46
2:A:400:TYR:CE2	2:A:402:ARG:HB2	2.51	0.46
1:B:950:G:O2'	1:B:951:A:H5'	2.16	0.46
1:B:916:C:H3'	1:B:916:C:OP2	2.16	0.46
1:B:923:G:O2'	1:B:924:G:H5'	2.16	0.45
2:A:351:LEU:HD23	2:A:351:LEU:C	2.37	0.45
2:A:422:VAL:HG22	2:A:430:ILE:HG23	1.98	0.45
1:B:936:G:C4	2:A:401:LYS:HD3	2.51	0.45
2:A:302:THR:OG1	2:A:305:SER:HB3	2.16	0.45
1:B:961:C:H2'	1:B:962:C:C6	2.50	0.45
2:A:270:LYS:N	5:A:1505:HOH:O	2.49	0.45
2:A:369:PRO:O	2:A:371:LYS:N	2.49	0.45
2:A:377:ARG:HG2	2:A:377:ARG:NH1	2.32	0.45
2:A:427:GLU:O	2:A:427:GLU:HG2	2.16	0.45
2:A:403:LEU:CA	2:A:409:VAL:HG11	2.47	0.45
1:B:935:U:C2	2:A:519:GLU:HG3	2.53	0.44
1:B:963:U:O2'	1:B:964:C:H5'	2.17	0.44
2:A:30:ARG:NH1	2:A:215:HIS:NE2	2.66	0.44
2:A:105:GLN:HG2	2:A:221:LEU:HD11	1.99	0.44
2:A:199:HIS:ND1	2:A:200:GLN:HG2	2.32	0.44
2:A:403:LEU:N	2:A:409:VAL:HG11	2.32	0.44
2:A:521:GLU:OE2	2:A:521:GLU:HA	2.17	0.44
2:A:105:GLN:HG2	2:A:221:LEU:CD1	2.48	0.44
1:B:916:C:O2'	1:B:918:G:OP2	2.28	0.44
1:B:967:A:H2'	1:B:968:C:H6	1.82	0.44
2:A:403:LEU:HA	2:A:409:VAL:CG1	2.48	0.44
2:A:227:SER:OG	2:A:229:ARG:NH1	2.51	0.43
2:A:407:LYS:CG	2:A:408:GLU:N	2.81	0.43
2:A:270:LYS:O	2:A:274:ASN:HB2	2.18	0.43
2:A:365:MET:HG2	2:A:413:ASN:CB	2.48	0.43
1:B:934:C:O2'	2:A:412:ARG:NH1	2.51	0.43
2:A:225:THR:OG1	2:A:226:HIS:CD2	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:526:LEU:CG	2:A:527:ASP:N	2.78	0.43
2:A:87:TRP:CE2	2:A:297:ARG:HD3	2.54	0.43
2:A:174:ALA:O	2:A:187:ASP:HA	2.19	0.43
2:A:183:ILE:HA	2:A:186:ARG:HG3	2.00	0.43
1:B:958:A:O2'	1:B:959:A:H3'	2.19	0.43
2:A:229:ARG:O	2:A:257:GLU:HA	2.19	0.42
2:A:407:LYS:CD	2:A:408:GLU:H	2.32	0.42
2:A:225:THR:OG1	2:A:226:HIS:HD2	2.02	0.42
2:A:39:LEU:HA	2:A:43:HIS:ND1	2.35	0.42
2:A:397:ASN:HB2	2:A:398:LYS:H	1.65	0.42
2:A:407:LYS:CG	2:A:408:GLU:H	2.32	0.42
2:A:474:ARG:HD2	5:A:1484:HOH:O	2.18	0.42
2:A:270:LYS:HG2	5:A:1505:HOH:O	2.19	0.42
1:B:919:G:C4	1:B:957:G:N2	2.88	0.42
2:A:393:ARG:O	2:A:404:VAL:HA	2.19	0.42
2:A:467:VAL:HG12	2:A:469:ILE:HG13	2.02	0.42
1:B:919:G:C5	1:B:957:G:N2	2.88	0.42
1:B:921:A:H62	1:B:947:U:H1'	1.84	0.42
2:A:45:LYS:HD3	4:A:998:QSI:H2	2.01	0.42
2:A:418:LYS:HG2	2:A:419:ALA:O	2.20	0.42
2:A:231:LEU:HD12	2:A:231:LEU:HA	1.89	0.42
2:A:136:LEU:CD2	2:A:183:ILE:HD11	2.40	0.41
2:A:391:ASP:HB3	2:A:456:ILE:HG21	2.02	0.41
1:B:935:U:O3'	2:A:520:ARG:HD2	2.21	0.41
2:A:230:THR:HG21	2:A:260:ARG:HB3	2.01	0.41
2:A:407:LYS:HD2	2:A:408:GLU:H	1.85	0.41
2:A:545:ARG:NH2	2:A:547:THR:HG21	2.35	0.41
2:A:404:VAL:O	2:A:406:GLY:N	2.54	0.41
1:B:967:A:H2'	1:B:968:C:O4'	2.21	0.41
2:A:182:PHE:CZ	2:A:238:ARG:HD3	2.56	0.41
2:A:457:HIS:HE1	5:A:1457:HOH:O	2.02	0.41
2:A:512:ALA:CB	2:A:527:ASP:HB2	2.51	0.41
2:A:281:HIS:HE1	5:A:1475:HOH:O	2.04	0.41
1:B:903:G:C2'	1:B:904:G:H5'	2.51	0.40
2:A:343:MET:HE1	2:A:412:ARG:HB3	2.03	0.40
2:A:230:THR:CB	2:A:232:GLU:OE1	2.68	0.40
2:A:207:ILE:O	2:A:207:ILE:HG13	2.21	0.40
2:A:349:VAL:HB	2:A:389:ARG:HG2	2.04	0.40
2:A:403:LEU:HD13	2:A:409:VAL:CG2	2.44	0.40
2:A:512:ALA:HB1	2:A:527:ASP:HB2	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	525/556 (94%)	487 (93%)	28 (5%)	10 (2%)	8 15

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	405	LEU
2	A	370	ASN
2	A	397	ASN
2	A	396	ALA
2	A	32	PRO
2	A	369	PRO
2	A	426	ALA
2	A	427	GLU
2	A	526	LEU
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	463/486 (95%)	424 (92%)	39 (8%)	11 21

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	30	ARG

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Mol	Chain	Res	Type
2	A	32	PRO
2	A	39	LEU
2	A	40	HIS
2	A	49	LEU
2	A	78	VAL
2	A	105	GLN
2	A	106	LEU
2	A	124	LEU
2	A	154	LEU
2	A	156	LEU
2	A	184	VAL
2	A	186	ARG
2	A	190	LEU
2	A	192	ARG
2	A	229	ARG
2	A	231	LEU
2	A	232	GLU
2	A	234	GLN
2	A	263	LEU
2	A	282	VAL
2	A	322	ILE
2	A	327	LEU
2	A	335	LEU
2	A	341	ARG
2	A	378	GLN
2	A	395	GLU
2	A	398	LYS
2	A	410	ARG
2	A	422	VAL
2	A	432	THR
2	A	437	TYR
2	A	441	THR
2	A	475	LEU
2	A	490	VAL
2	A	497	VAL
2	A	506	SER
2	A	519	GLU
2	A	528	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	28	HIS
2	A	115	ASN
2	A	128	GLN
2	A	142	ASN
2	A	153	ASN
2	A	226	HIS
2	A	234	GLN
2	A	236	ASN
2	A	255	GLN
2	A	281	HIS
2	A	318	GLN
2	A	368	HIS
2	A	429	ASN
2	A	457	HIS
2	A	530	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	73/75 (97%)	18 (24%)	9 (12%)

All (18) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	908	U
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	935	U
1	B	936	G
1	B	937	A
1	B	941	C
1	B	946	U
1	B	948	C
1	B	949	C
1	B	961	C
1	B	973	G
1	B	974	C
1	B	975	C

All (9) 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	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	SO4	A	1395	-	4,4,4	0.28	0	6,6,6	0.09	0
3	SO4	A	1394	-	4,4,4	0.16	0	6,6,6	0.09	0
4	QSI	A	998	-	31,34,34	1.26	5 (16%)	34,50,50	1.43	4 (11%)

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
4	QSI	A	998	-	-	5/19/40/40	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	998	QSI	C8-N7	-3.32	1.28	1.34
4	A	998	QSI	S-N10	3.23	1.65	1.59
4	A	998	QSI	O1S-S	-2.57	1.40	1.42
4	A	998	QSI	O5'-S	-2.47	1.54	1.59
4	A	998	QSI	O4'-C1'	2.15	1.44	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	998	QSI	N3-C2-N1	-4.74	121.27	128.68
4	A	998	QSI	C5'-O5'-S	-3.00	111.18	117.37
4	A	998	QSI	O4'-C4'-C3'	2.04	109.14	105.11
4	A	998	QSI	CG-CB-CA	-2.00	109.17	113.84

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	998	QSI	N-CA-CB-CG
4	A	998	QSI	C5'-O5'-S-N10
4	A	998	QSI	C3'-C4'-C5'-O5'
4	A	998	QSI	C-CA-CB-CG
4	A	998	QSI	O4'-C4'-C5'-O5'

There are no ring outliers.

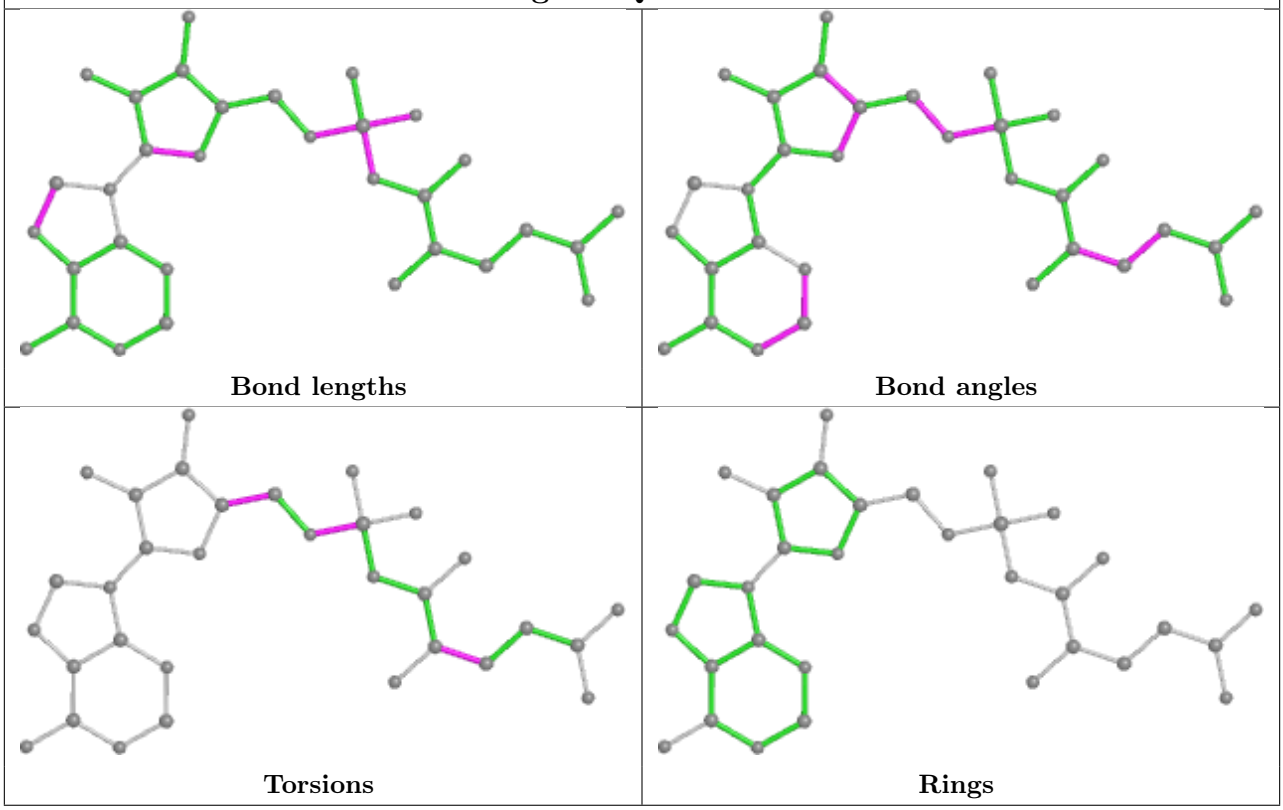
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	998	QSI	3	0

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

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

Ligand QSI A 998



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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.