



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 02:24 AM EDT

PDB ID : 1O0C
Title : CRYSTAL STRUCTURE OF L-GLUTAMATE AND AMPCPP BOUND TO
GLUTAMINE AMINOACYL TRNA SYNTHETASE
Authors : Bullock, T.L.; Perona, J.J.
Deposited on : 2003-02-20
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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)
Xtrriage (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

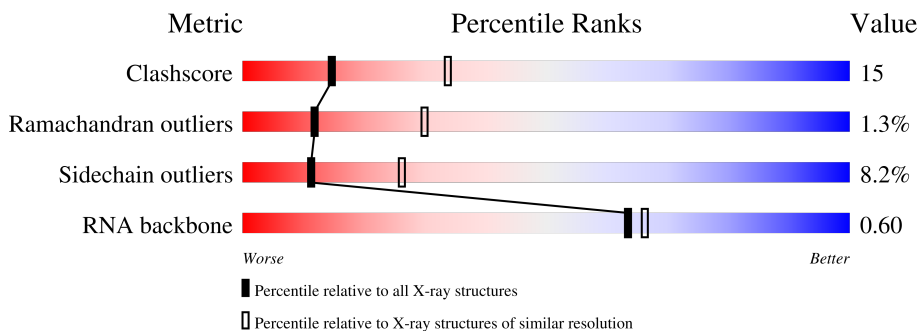
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RNA backbone	3102	1159 (3.00-2.40)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	75	
2	A	554	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GLU	A	996	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	AMP	A	998	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6036 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	74	1570	702	279	516	73	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	901	U	G	engineered mutation	EMBL 43058

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

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

There is a discrepancy between the modelled and reference sequences:

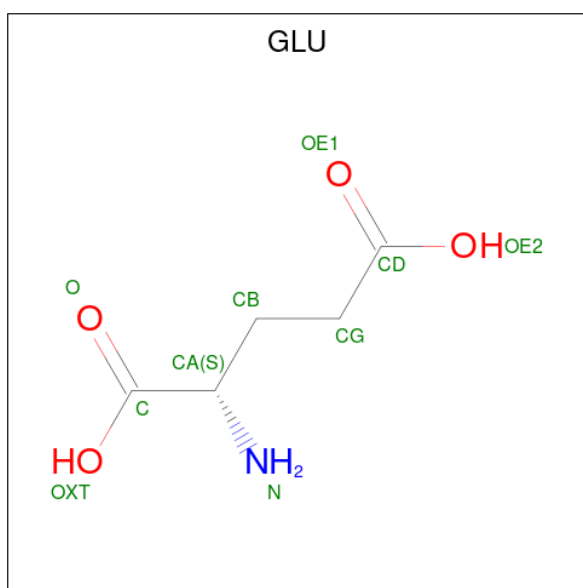
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	cloning artifact	UNP P00962

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



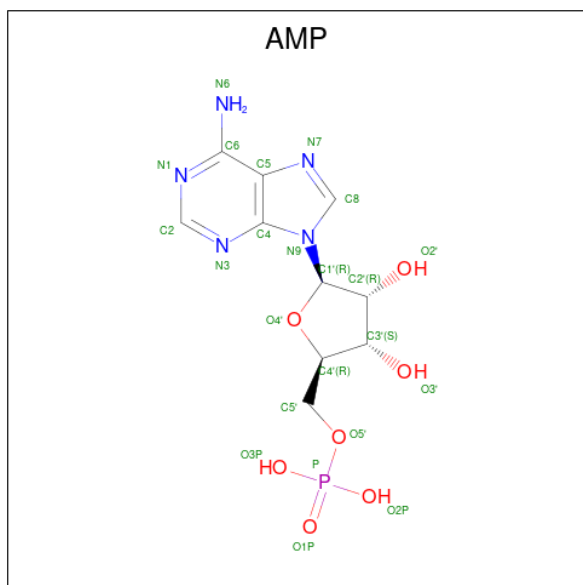
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 5 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	23	10	5	7	1	0	0

- Molecule 6 is water.

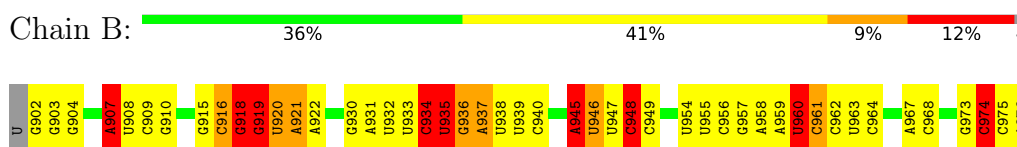
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	26	Total	O	0	0
			26	26		
6	A	118	Total	O	0	0
			118	118		

3 Residue-property plots [i](#)

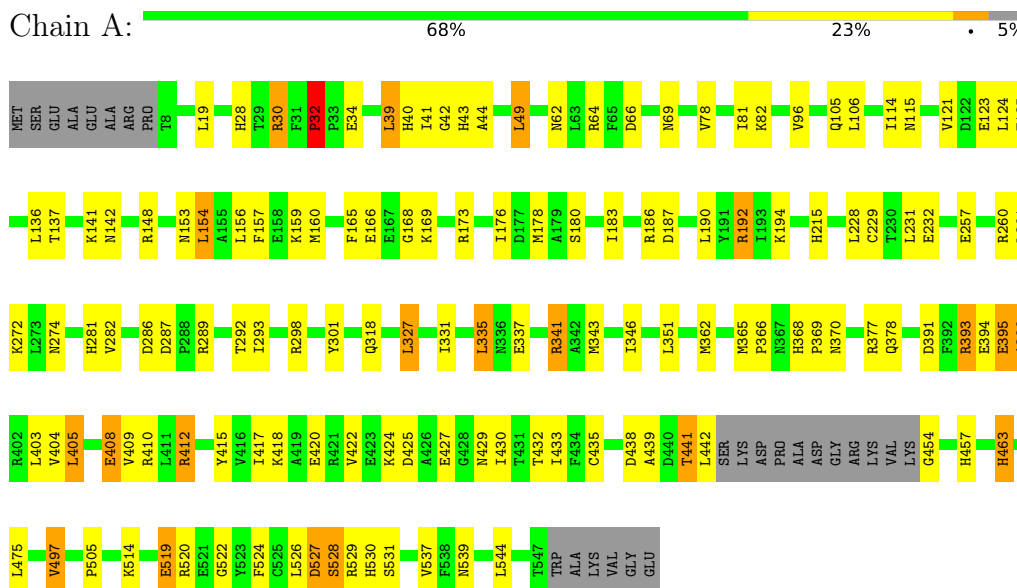
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: Glutaminyl tRNA



- Molecule 2: Glutaminyl-tRNA synthetase



4 Data and refinement statistics

Xtrriage (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	241.10Å 94.58Å 116.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.70)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 98.0	Depositor
R, R_{free}	0.213 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6036	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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, AMP

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	0.46	0/1753	0.88	8/2730 (0.3%)
2	A	0.44	0/4379	0.68	0/5928
All	All	0.44	0/6132	0.75	8/8658 (0.1%)

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 (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	919	G	N9-C1'-C2'	6.70	122.71	114.00
1	B	918	G	N9-C1'-C2'	6.46	122.39	114.00
1	B	936	G	N9-C1'-C2'	6.29	122.18	114.00
1	B	974	C	N1-C1'-C2'	5.95	121.74	114.00
1	B	945	A	N9-C1'-C2'	5.86	121.62	114.00
1	B	934	C	N1-C1'-C2'	5.42	121.04	114.00
1	B	948	C	N1-C1'-C2'	5.11	120.64	114.00
1	B	907	A	N9-C1'-C2'	5.04	120.55	114.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	919	G	Sidechain
1	B	935	U	Sidechain
1	B	948	C	Sidechain
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	60	0
2	A	4279	0	4172	112	0
3	A	10	0	0	2	0
4	A	10	0	5	4	0
5	A	23	0	10	2	0
6	A	118	0	0	6	0
6	B	26	0	0	0	0
All	All	6036	0	4988	163	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 15.

All (163) 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:946:U:H4'	1:B:947:U:C6	1.86	1.09
1:B:946:U:H4'	1:B:947:U:C5	1.95	1.01
2:A:531:SER:HB3	2:A:537:VAL:H	1.44	0.83
2:A:39:LEU:HD13	2:A:81:ILE:HG12	1.61	0.81
2:A:522:GLY:HA2	2:A:544:LEU:HD13	1.65	0.78
1:B:916:C:H3'	1:B:916:C:OP2	1.84	0.76
1:B:976:A:H4'	2:A:34:GLU:OE1	1.90	0.71
1:B:919:G:O2'	1:B:920:U:C6	2.44	0.70
1:B:946:U:C4'	1:B:947:U:C5	2.74	0.69
1:B:947:U:H2'	1:B:947:U:O2	1.93	0.68
1:B:960:U:H5'	1:B:961:C:OP2	1.94	0.67
2:A:471:LEU:HB2	2:A:497:VAL:HG13	1.77	0.65
1:B:930:G:O2'	1:B:931:A:H5'	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:939:U:O2'	1:B:940:C:H5'	1.98	0.64
2:A:125:THR:HG23	2:A:128:GLN:NE2	2.13	0.64
1:B:919:G:O2'	1:B:920:U:H6	1.78	0.63
2:A:341:ARG:HD3	2:A:369:PRO:HD2	1.80	0.62
1:B:960:U:H5''	1:B:961:C:H5	1.65	0.62
2:A:159:LYS:HD2	2:A:165:PHE:CE2	2.35	0.62
1:B:919:G:HO2'	1:B:920:U:H6	1.37	0.62
1:B:921:A:H62	1:B:947:U:H1'	1.64	0.61
2:A:125:THR:HG23	2:A:128:GLN:HE21	1.64	0.61
1:B:919:G:C4	1:B:957:G:N2	2.69	0.60
2:A:82:LYS:HD3	2:A:96:VAL:HG21	1.83	0.60
2:A:136:LEU:HD23	2:A:183:ILE:HD11	1.82	0.59
1:B:934:C:N4	2:A:410:ARG:HH21	2.00	0.59
1:B:963:U:H2'	1:B:964:C:C6	2.37	0.59
2:A:398:LYS:H	2:A:398:LYS:HD2	1.68	0.59
2:A:32:PRO:HA	2:A:64:ARG:O	2.03	0.58
2:A:173:ARG:HD2	2:A:187:ASP:O	2.04	0.58
2:A:393:ARG:O	2:A:404:VAL:HA	2.04	0.58
2:A:341:ARG:HB3	6:A:1494:HOH:O	2.04	0.58
2:A:166:GLU:O	2:A:169:LYS:HB2	2.04	0.57
4:A:996:GLU:O	5:A:998:AMP:H3'	2.04	0.57
1:B:937:A:C2	1:B:938:U:H1'	2.38	0.57
1:B:918:G:O2'	1:B:957:G:N2	2.38	0.56
2:A:40:HIS:HA	2:A:292:THR:HA	1.86	0.56
1:B:967:A:H2'	1:B:968:C:C6	2.40	0.56
1:B:935:U:O4	2:A:341:ARG:NH1	2.38	0.56
2:A:341:ARG:N	2:A:341:ARG:HD2	2.20	0.56
1:B:958:A:O2'	1:B:960:U:C6	2.57	0.56
1:B:939:U:C2'	1:B:940:C:H5'	2.36	0.55
1:B:916:C:C5'	1:B:960:U:O2	2.55	0.55
2:A:519:GLU:HB2	6:A:1494:HOH:O	2.06	0.55
1:B:958:A:HO2'	1:B:960:U:H6	1.49	0.55
1:B:958:A:HO2'	1:B:960:U:H5	1.49	0.54
2:A:229:CYS:O	2:A:257:GLU:HA	2.05	0.54
2:A:229:CYS:HB3	4:A:996:GLU:OE1	2.07	0.54
1:B:962:C:O2'	1:B:963:U:H5'	2.08	0.54
1:B:947:U:O2	1:B:947:U:C2'	2.56	0.54
2:A:272:LYS:HD2	3:A:1395:SO4:O1	2.07	0.54
2:A:123:GLU:HG3	2:A:148:ARG:HH22	1.72	0.53
2:A:331:ILE:HG13	2:A:335:LEU:HD22	1.90	0.53
2:A:526:LEU:HG	2:A:527:ASP:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:368:HIS:HD2	2:A:370:ASN:H	1.55	0.53
1:B:958:A:O2'	1:B:960:U:C5	2.59	0.52
2:A:40:HIS:CD2	6:A:1512:HOH:O	2.62	0.52
2:A:415:TYR:CE1	2:A:442:LEU:HD22	2.45	0.52
1:B:956:C:H2'	1:B:957:G:O4'	2.09	0.52
1:B:960:U:H5''	1:B:961:C:C5	2.45	0.52
2:A:403:LEU:HD13	2:A:409:VAL:HG22	1.92	0.52
2:A:526:LEU:HD12	2:A:537:VAL:O	2.10	0.52
2:A:438:ASP:HB3	2:A:441:THR:OG1	2.10	0.52
1:B:934:C:O2'	2:A:412:ARG:NH1	2.43	0.51
2:A:136:LEU:HD23	2:A:183:ILE:CD1	2.40	0.51
2:A:346:ILE:HG13	2:A:469:ILE:HD12	1.93	0.51
1:B:934:C:H41	2:A:410:ARG:HH21	1.57	0.51
2:A:346:ILE:HG13	2:A:469:ILE:CD1	2.40	0.51
1:B:907:A:H5'	2:A:318:GLN:NE2	2.25	0.51
2:A:132:TYR:CD2	2:A:141:LYS:HG3	2.45	0.51
2:A:287:ASP:OD1	2:A:289:ARG:HG3	2.11	0.51
2:A:28:HIS:HE1	2:A:62:ASN:OD1	1.94	0.51
2:A:394:GLU:HA	2:A:405:LEU:HB2	1.93	0.51
2:A:270:LYS:N	6:A:1512:HOH:O	2.43	0.50
1:B:933:U:H2'	1:B:935:U:OP1	2.12	0.50
2:A:301:TYR:CE2	2:A:327:LEU:HD22	2.46	0.50
2:A:142:ASN:HD22	2:A:178:MET:HG3	1.77	0.50
2:A:463:HIS:O	2:A:505:PRO:HD3	2.11	0.50
1:B:937:A:H2'	1:B:938:U:O4'	2.11	0.50
2:A:433:ILE:HG22	2:A:435:CYS:SG	2.52	0.50
1:B:902:G:C8	2:A:137:THR:HG22	2.47	0.50
2:A:30:ARG:NH2	2:A:228:LEU:O	2.45	0.50
2:A:281:HIS:HE1	6:A:1483:HOH:O	1.94	0.49
1:B:915:G:H2'	1:B:959:A:N1	2.28	0.49
2:A:395:GLU:O	2:A:396:ALA:HB3	2.13	0.49
2:A:157:PHE:O	2:A:160:MET:HB2	2.12	0.49
2:A:341:ARG:HD3	2:A:369:PRO:CD	2.42	0.49
2:A:183:ILE:HA	2:A:186:ARG:HG3	1.94	0.49
1:B:916:C:H5''	1:B:960:U:O2	2.13	0.48
1:B:921:A:N6	1:B:947:U:O2'	2.47	0.48
2:A:229:CYS:SG	2:A:257:GLU:HG3	2.53	0.48
1:B:939:U:H2'	1:B:940:C:O4'	2.14	0.48
1:B:903:G:O2'	1:B:904:G:H5'	2.14	0.48
1:B:935:U:H5'	2:A:412:ARG:HH12	1.79	0.48
2:A:114:ILE:HG21	2:A:154:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:180:SER:O	2:A:186:ARG:NH1	2.47	0.47
1:B:916:C:H5'	1:B:960:U:O2	2.15	0.47
2:A:341:ARG:HD2	2:A:341:ARG:H	1.79	0.47
2:A:301:TYR:HE2	2:A:327:LEU:HD22	1.79	0.47
2:A:377:ARG:HH11	2:A:377:ARG:HG2	1.80	0.47
2:A:393:ARG:HB2	2:A:400:TYR:CZ	2.50	0.47
2:A:522:GLY:HA2	2:A:544:LEU:CD1	2.42	0.47
2:A:474:ARG:HD2	6:A:1491:HOH:O	2.15	0.47
1:B:921:A:C2	1:B:948:C:C2	3.03	0.47
2:A:123:GLU:CG	2:A:148:ARG:HH22	2.27	0.47
2:A:282:VAL:HG12	2:A:289:ARG:NH1	2.30	0.46
1:B:974:C:N3	2:A:168:GLY:HA2	2.30	0.46
1:B:963:U:H2'	1:B:964:C:O4'	2.16	0.46
2:A:529:ARG:HA	2:A:529:ARG:HE	1.80	0.46
2:A:114:ILE:CG2	2:A:154:LEU:HD13	2.45	0.46
1:B:932:U:C4	1:B:933:U:C4	3.03	0.46
2:A:121:VAL:H	2:A:153:ASN:ND2	2.13	0.45
2:A:362:MET:HG3	2:A:378:GLN:HG3	1.99	0.45
2:A:365:MET:HA	2:A:366:PRO:HD3	1.82	0.45
2:A:343:MET:HE1	2:A:457:HIS:HA	1.98	0.45
2:A:528:SER:O	2:A:530:HIS:CD2	2.70	0.45
1:B:957:G:H2'	1:B:958:A:H5'	1.98	0.45
2:A:408:GLU:HA	2:A:417:ILE:O	2.17	0.45
2:A:260:ARG:HB2	5:A:998:AMP:C6	2.52	0.45
2:A:32:PRO:HG2	4:A:996:GLU:HB3	1.98	0.44
2:A:30:ARG:NH1	2:A:215:HIS:NE2	2.64	0.44
2:A:362:MET:CG	2:A:378:GLN:HG3	2.47	0.44
2:A:457:HIS:H	2:A:457:HIS:CD2	2.35	0.44
2:A:141:LYS:O	2:A:178:MET:HE2	2.18	0.44
2:A:457:HIS:HD2	2:A:520:ARG:HE	1.65	0.44
2:A:229:CYS:HB3	4:A:996:GLU:CD	2.38	0.43
2:A:115:ASN:HD21	2:A:154:LEU:HD21	1.82	0.43
1:B:915:G:O2'	1:B:959:A:N6	2.48	0.43
1:B:955:U:O5'	1:B:955:U:H6	2.02	0.43
2:A:410:ARG:HH21	2:A:442:LEU:HA	1.84	0.43
2:A:401:LYS:O	2:A:454:GLY:HA3	2.19	0.43
1:B:920:U:O2	1:B:920:U:C2'	2.67	0.43
2:A:125:THR:CG2	2:A:128:GLN:HE21	2.30	0.43
1:B:947:U:O2'	1:B:948:C:C6	2.65	0.43
2:A:394:GLU:HG2	2:A:405:LEU:HD22	2.01	0.43
1:B:915:G:HO2'	1:B:916:C:P	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:920:U:O2	1:B:920:U:H2'	2.17	0.43
1:B:935:U:O3'	2:A:520:ARG:HD2	2.19	0.43
2:A:346:ILE:N	2:A:346:ILE:HD12	2.34	0.42
2:A:270:LYS:O	2:A:274:ASN:HB2	2.19	0.42
2:A:351:LEU:C	2:A:351:LEU:HD23	2.40	0.42
2:A:527:ASP:CG	2:A:529:ARG:H	2.22	0.42
2:A:424:LYS:HA	2:A:430:ILE:HA	2.00	0.42
2:A:427:GLU:O	2:A:427:GLU:HG2	2.19	0.42
2:A:286:ASP:O	2:A:298:ARG:HD3	2.20	0.42
2:A:391:ASP:OD1	2:A:520:ARG:NH2	2.53	0.42
2:A:422:VAL:HG23	2:A:433:ILE:HG13	2.02	0.42
1:B:919:G:C5	1:B:957:G:N2	2.88	0.42
2:A:44:ALA:HB2	2:A:293:ILE:HD11	2.02	0.42
1:B:954:U:C4	1:B:955:U:C4	3.08	0.41
2:A:377:ARG:HG2	2:A:377:ARG:NH1	2.35	0.41
2:A:418:LYS:HD2	2:A:420:GLU:OE2	2.20	0.41
2:A:49:LEU:HD13	2:A:228:LEU:HD13	2.02	0.41
2:A:474:ARG:HE	2:A:474:ARG:HB3	1.70	0.41
2:A:69:ASN:OD1	2:A:194:LYS:NZ	2.52	0.41
2:A:526:LEU:CG	2:A:527:ASP:H	2.34	0.41
1:B:945:A:HO2'	1:B:946:U:P	2.44	0.41
2:A:42:GLY:HA2	2:A:261:LEU:HD23	2.02	0.41
2:A:43:HIS:NE2	3:A:1394:SO4:O4	2.54	0.41
2:A:524:PHE:HA	2:A:539:ASN:O	2.20	0.41
2:A:425:ASP:OD1	2:A:429:ASN:N	2.54	0.40
1:B:958:A:O2'	1:B:960:U:H6	1.99	0.40
2:A:192:ARG:HD3	2:A:194:LYS:HE3	2.03	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	525/554 (95%)	500 (95%)	18 (3%)	7 (1%)	12 30

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	397	ASN
2	A	405	LEU
2	A	32	PRO
2	A	396	ALA
2	A	527	ASP
2	A	439	ALA
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	463/482 (96%)	426 (92%)	37 (8%)	12 27

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	19	LEU
2	A	30	ARG
2	A	32	PRO
2	A	39	LEU
2	A	41	ILE
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

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Mol	Chain	Res	Type
2	A	190	LEU
2	A	192	ARG
2	A	231	LEU
2	A	232	GLU
2	A	263	LEU
2	A	327	LEU
2	A	335	LEU
2	A	337	GLU
2	A	341	ARG
2	A	393	ARG
2	A	395	GLU
2	A	397	ASN
2	A	398	LYS
2	A	408	GLU
2	A	412	ARG
2	A	432	THR
2	A	441	THR
2	A	463	HIS
2	A	475	LEU
2	A	497	VAL
2	A	514	LYS
2	A	519	GLU
2	A	528	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) 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	236	ASN
2	A	281	HIS
2	A	355	ASN
2	A	368	HIS
2	A	378	GLN
2	A	457	HIS
2	A	530	HIS

5.3.3 RNA 

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	73/75 (97%)	21 (28%)	13 (17%)

All (21) 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	922	A
1	B	934	C
1	B	935	U
1	B	936	G
1	B	937	A
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 (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	934	C
1	B	935	U
1	B	936	G
1	B	945	A
1	B	948	C
1	B	960	U

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Mol	Chain	Res	Type
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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	1395	-	4,4,4	0.80	0	6,6,6	0.60	0
5	AMP	A	998	-	22,25,25	2.03	6 (27%)	25,38,38	1.57	4 (16%)
3	SO4	A	1394	-	4,4,4	0.77	0	6,6,6	0.53	0
4	GLU	A	996	-	2,9,9	0.35	0	2,11,11	0.58	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	AMP	A	998	-	1/1/5/5	4/6/26/26	0/3/3/3
4	GLU	A	996	-	-	1/3/9/9	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	998	AMP	O2'-C2'	-7.17	1.26	1.43
5	A	998	AMP	P-O5'	-2.51	1.52	1.60
5	A	998	AMP	C2-N3	2.47	1.36	1.32
5	A	998	AMP	C8-N7	-2.41	1.30	1.34
5	A	998	AMP	O5'-C5'	2.15	1.53	1.44
5	A	998	AMP	P-O2P	-2.13	1.46	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	998	AMP	O4'-C1'-C2'	4.18	113.04	106.93
5	A	998	AMP	O3P-P-O2P	-2.65	97.50	107.64
5	A	998	AMP	O3P-P-O1P	2.26	119.55	110.68
5	A	998	AMP	O2P-P-O1P	2.11	118.96	110.68

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	998	AMP	C1'

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	996	GLU	CA-CB-CG-CD
5	A	998	AMP	C5'-O5'-P-O1P
5	A	998	AMP	C5'-O5'-P-O3P
5	A	998	AMP	O4'-C4'-C5'-O5'
5	A	998	AMP	C3'-C4'-C5'-O5'

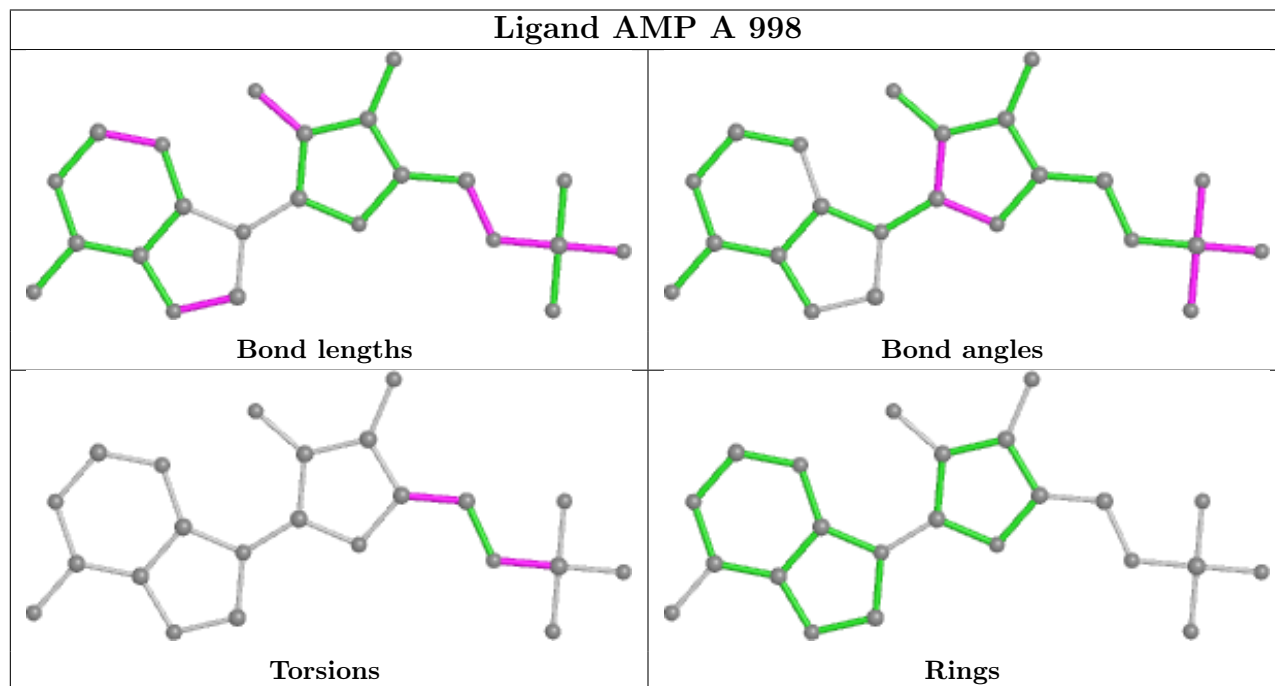
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1395	SO4	1	0
5	A	998	AMP	2	0
3	A	1394	SO4	1	0
4	A	996	GLU	4	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.