



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:26 AM UTC

PDB ID : 1ZJW / pdb_00001zjw
Title : Glutaminyl-tRNA synthetase complexed to glutamine and 2'deoxy A76 glutamine tRNA
Authors : Gruic-Sovulj, I.; Uter, N.; Bullock, T.; Perona, J.J.
Deposited on : 2005-05-01
Resolution : 2.50 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

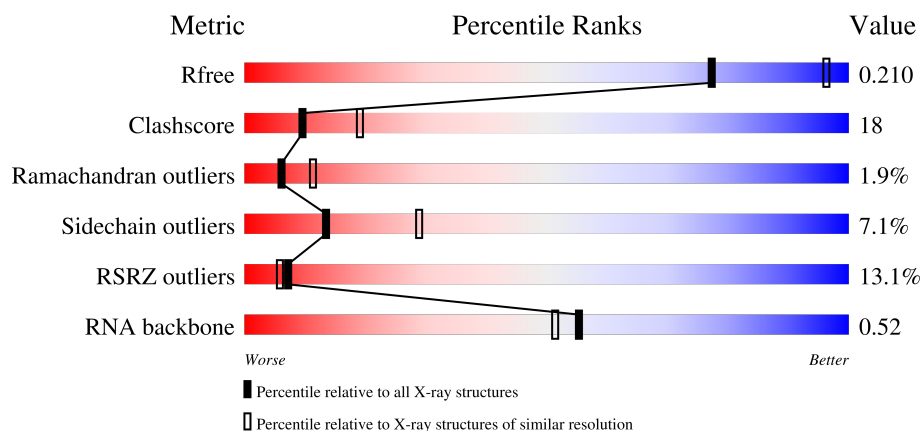
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)
RNA backbone	3983	1003 (2.78-2.22)

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	75	36% 47% 31% 12% 9%
2	A	553	9% 65% 24% 6%

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
5	GLN	A	996	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6033 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.

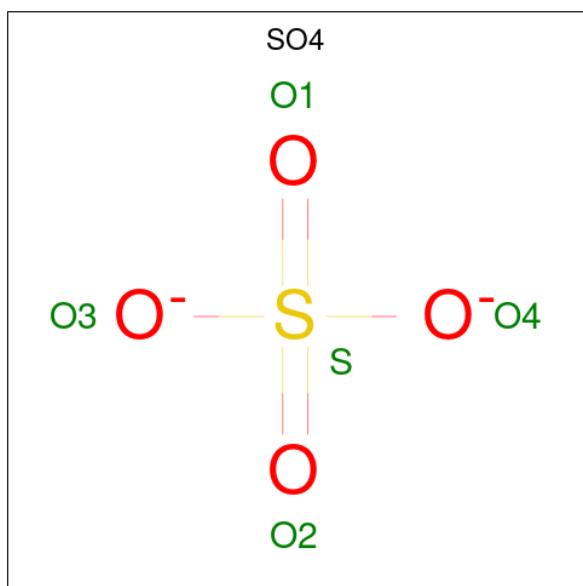
- Molecule 1 is a RNA chain called Glutaminyl-tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	74	Total	C	N	O	P	0	0	0
			1569	702	279	515	73			

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

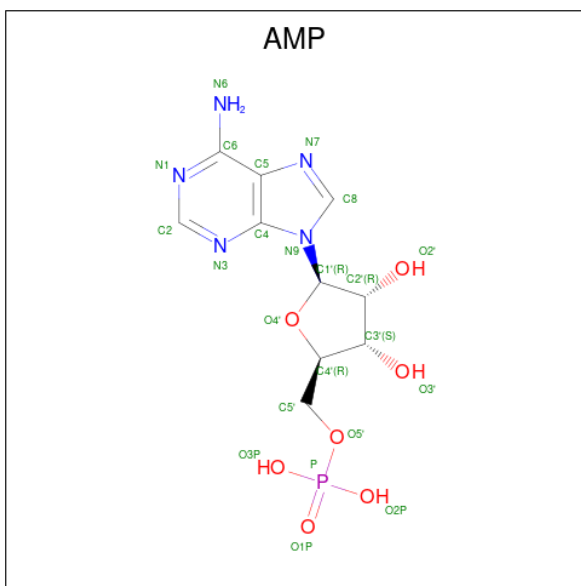
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	529	Total	C	N	O	S	0	0	0
			4279	2704	752	802	21			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



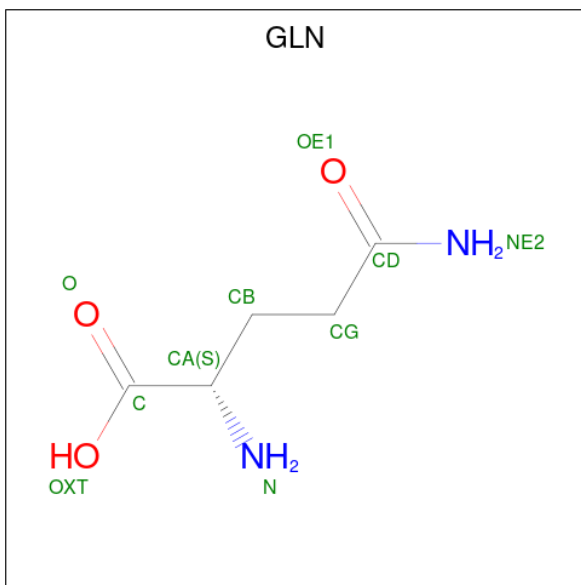
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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

- Molecule 5 is GLUTAMINE (CCD ID: GLN) (formula: $C_5H_{10}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			10	5	2	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	26	Total 26	O 26	0	0
6	A	116	Total 116	O 116	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	238.66Å 93.47Å 114.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.00 – 2.50 60.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (60.00-2.50) 99.5 (60.00-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.249 0.214 , 0.210	Depositor DCC
R_{free} test set	2861 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 75.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6033	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: 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	0.32	0/1752	0.80	8/2728 (0.3%)
2	A	0.45	0/4379	0.92	16/5928 (0.3%)
All	All	0.42	0/6131	0.89	24/8656 (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 (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	250	PRO	N-CA-C	8.14	124.04	113.86
1	B	976	A	C4'-C3'-O3'	7.62	121.43	110.00
2	A	231	LEU	N-CA-C	7.39	121.39	112.38
2	A	69	ASN	CA-C-N	7.23	127.56	119.32
2	A	69	ASN	C-N-CA	7.23	127.56	119.32
2	A	32	PRO	N-CA-C	7.17	119.45	110.70
1	B	909	C	C2'-C3'-O3'	-7.00	103.21	113.70
2	A	215	HIS	N-CA-C	6.69	118.23	111.07
2	A	348	PRO	N-CA-C	6.67	121.66	111.19
1	B	936	G	N9-C1'-C2'	6.62	121.94	112.00
2	A	478	VAL	CA-C-N	5.93	125.63	119.05
2	A	478	VAL	C-N-CA	5.93	125.63	119.05
2	A	249	ILE	CA-C-N	5.87	125.49	119.56
2	A	249	ILE	C-N-CA	5.87	125.49	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	974	C	C4'-C3'-O3'	-5.80	100.70	109.40
2	A	124	LEU	N-CA-C	-5.76	101.76	110.28
1	B	916	C	C2'-C3'-O3'	5.72	118.08	109.50
1	B	948	C	C4'-C3'-O3'	-5.61	104.59	113.00
1	B	974	C	N1-C1'-C2'	5.58	122.38	114.00
2	A	214	THR	N-CA-C	5.56	117.14	111.14
2	A	206	CYS	N-CA-C	-5.38	105.54	113.61
1	B	936	G	C4'-C3'-O3'	-5.33	105.00	113.00
2	A	63	LEU	N-CA-C	-5.14	100.14	108.52
2	A	498	ILE	N-CA-C	5.04	115.34	107.99

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	919	G	Sidechain
1	B	936	G	Sidechain
1	B	960	U	Sidechain
1	B	974	C	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1569	0	801	46	0
2	A	4279	0	4172	151	0
3	A	10	0	0	0	0
4	A	23	0	12	3	0
5	A	10	0	7	7	0
6	A	116	0	0	8	0
6	B	26	0	0	0	0
All	All	6033	0	4992	190	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 18.

All (190) 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:136:LEU:HD23	2:A:183:ILE:HD11	1.53	0.89
4:A:998:AMP:O3'	5:A:996:GLN:HB2	1.74	0.87
2:A:393:ARG:HG2	2:A:396:ALA:HB2	1.57	0.86
2:A:471:LEU:HB2	2:A:497:VAL:HG13	1.58	0.85
2:A:529:ARG:HA	2:A:529:ARG:HE	1.42	0.82
1:B:909:C:H5''	1:B:910:G:OP2	1.85	0.76
2:A:192:ARG:CD	2:A:194:LYS:HE3	2.16	0.74
2:A:526:LEU:HG	2:A:527:ASP:H	1.52	0.74
1:B:946:U:H4'	1:B:947:U:C6	2.23	0.72
2:A:343:MET:HE1	2:A:412:ARG:HB3	1.71	0.71
1:B:934:C:O2'	2:A:455:VAL:HG21	1.90	0.71
2:A:341:ARG:HB3	6:A:1493:HOH:O	1.91	0.71
2:A:403:LEU:HD13	2:A:409:VAL:HG22	1.72	0.71
1:B:946:U:H4'	1:B:947:U:C5	2.26	0.71
2:A:504:GLU:HG3	2:A:506:SER:HB3	1.73	0.70
1:B:974:C:N3	2:A:168:GLY:HA2	2.05	0.70
2:A:471:LEU:HB2	2:A:497:VAL:CG1	2.20	0.70
2:A:39:LEU:HD13	2:A:81:ILE:HG12	1.74	0.69
2:A:522:GLY:HA2	2:A:544:LEU:HD13	1.73	0.69
1:B:934:C:O2'	1:B:935:U:H5'	1.93	0.68
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:362:MET:CG	2:A:378:GLN:HG3	2.24	0.67
1:B:935:U:O2'	2:A:520:ARG:HG2	1.94	0.66
1:B:976:A:H2''	5:A:996:GLN:HA	1.76	0.66
1:B:958:A:HO2'	1:B:960:U:H5	1.43	0.66
2:A:212:ASP:HB3	2:A:239:LEU:HD23	1.78	0.66
2:A:136:LEU:HD23	2:A:183:ILE:CD1	2.25	0.66
2:A:534:GLU:H	2:A:534:GLU:CD	2.03	0.66
1:B:935:U:O4	2:A:341:ARG:NH1	2.30	0.65
2:A:280:LYS:HD2	6:A:1504:HOH:O	1.96	0.65
2:A:397:ASN:ND2	2:A:399:GLN:HB2	2.11	0.65
2:A:393:ARG:O	2:A:404:VAL:HA	1.96	0.65
2:A:512:ALA:HA	2:A:526:LEU:HB3	1.80	0.64
1:B:934:C:HO2'	2:A:455:VAL:HG21	1.63	0.63
2:A:403:LEU:N	2:A:409:VAL:HG11	2.14	0.63
2:A:124:LEU:HD12	2:A:128:GLN:NE2	2.14	0.62
2:A:270:LYS:N	6:A:1511:HOH:O	2.31	0.62
2:A:121:VAL:H	2:A:153:ASN:ND2	1.98	0.62
1:B:930:G:O2'	1:B:931:A:H5'	2.00	0.61
2:A:159:LYS:HD2	2:A:165:PHE:CE2	2.35	0.61
2:A:529:ARG:HA	2:A:529:ARG:NE	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:351:LEU:C	2:A:351:LEU:HD23	2.25	0.61
2:A:398:LYS:H	2:A:398:LYS:HD2	1.66	0.61
1:B:921:A:N6	1:B:947:U:H1'	2.16	0.60
2:A:30:ARG:NH2	2:A:228:LEU:O	2.34	0.60
2:A:362:MET:HG2	2:A:378:GLN:HG3	1.82	0.60
2:A:343:MET:HE3	2:A:458:TRP:H	1.67	0.60
2:A:397:ASN:HD21	2:A:399:GLN:HB2	1.67	0.60
1:B:963:U:H2'	1:B:964:C:C6	2.37	0.59
2:A:442:LEU:HD23	2:A:442:LEU:N	2.17	0.59
2:A:512:ALA:HB1	2:A:527:ASP:HB2	1.85	0.59
2:A:192:ARG:HD3	2:A:194:LYS:HE3	1.84	0.59
2:A:124:LEU:HA	2:A:128:GLN:NE2	2.18	0.59
2:A:40:HIS:HA	2:A:292:THR:HA	1.85	0.58
2:A:438:ASP:HB3	2:A:441:THR:OG1	2.03	0.58
2:A:212:ASP:CB	2:A:239:LEU:HD23	2.33	0.58
1:B:918:G:O2'	1:B:957:G:N2	2.38	0.57
2:A:211:TYR:HE1	5:A:996:GLN:HG2	1.69	0.57
2:A:422:VAL:HG22	2:A:423:GLU:H	1.70	0.57
2:A:301:TYR:CE2	2:A:327:LEU:HD22	2.40	0.56
4:A:998:AMP:H3'	5:A:996:GLN:O	2.06	0.56
2:A:301:TYR:HE2	2:A:327:LEU:HD22	1.71	0.56
2:A:231:LEU:HD13	2:A:258:PHE:C	2.30	0.56
2:A:199:HIS:ND1	2:A:200:GLN:HG2	2.21	0.55
2:A:173:ARG:HD2	2:A:187:ASP:O	2.06	0.55
2:A:159:LYS:HD2	2:A:165:PHE:CD2	2.42	0.55
1:B:921:A:H62	1:B:947:U:H1'	1.72	0.55
2:A:32:PRO:HA	2:A:64:ARG:O	2.07	0.54
1:B:962:C:O2'	1:B:963:U:H5'	2.07	0.54
1:B:947:U:O2	1:B:947:U:C2'	2.55	0.54
2:A:527:ASP:CG	2:A:529:ARG:H	2.15	0.54
2:A:410:ARG:HD3	2:A:416:VAL:HG22	1.90	0.53
2:A:526:LEU:HG	2:A:527:ASP:N	2.21	0.53
1:B:939:U:H2'	1:B:940:C:O4'	2.09	0.53
1:B:961:C:H2'	1:B:962:C:H6	1.74	0.53
2:A:424:LYS:HD3	2:A:428:GLY:O	2.09	0.53
2:A:341:ARG:N	2:A:341:ARG:HD2	2.25	0.53
1:B:916:C:O2'	1:B:918:G:OP2	2.26	0.52
2:A:121:VAL:H	2:A:153:ASN:HD22	1.57	0.52
2:A:391:ASP:OD1	2:A:520:ARG:NH2	2.43	0.52
2:A:425:ASP:OD1	2:A:429:ASN:HB2	2.10	0.52
1:B:908:U:O4'	1:B:948:C:O2'	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:393:ARG:HD3	2:A:400:TYR:CZ	2.45	0.52
2:A:395:GLU:OE1	2:A:395:GLU:N	2.42	0.52
1:B:919:G:N2	1:B:957:G:H1'	2.25	0.52
2:A:391:ASP:OD1	2:A:402:ARG:HD2	2.10	0.52
2:A:402:ARG:C	2:A:409:VAL:HG11	2.35	0.52
2:A:273:LEU:O	2:A:277:VAL:HG23	2.10	0.52
2:A:528:SER:C	2:A:530:HIS:H	2.18	0.51
2:A:211:TYR:CE1	5:A:996:GLN:HG2	2.45	0.51
1:B:976:A:H4'	2:A:34:GLU:OE1	2.10	0.51
2:A:125:THR:H	2:A:128:GLN:NE2	2.09	0.51
1:B:919:G:C4	1:B:957:G:N2	2.79	0.51
2:A:511:VAL:HG23	2:A:514:LYS:HB3	1.94	0.50
2:A:346:ILE:HG12	2:A:469:ILE:CD1	2.42	0.50
2:A:412:ARG:HD3	2:A:413:ASN:N	2.27	0.50
2:A:357:GLN:H	2:A:357:GLN:CD	2.20	0.50
1:B:918:G:H2'	1:B:957:G:H22	1.76	0.50
1:B:960:U:H5''	1:B:961:C:H5	1.77	0.49
2:A:398:LYS:HD2	2:A:398:LYS:N	2.27	0.49
1:B:935:U:C2	2:A:519:GLU:HG2	2.48	0.48
2:A:365:MET:HG2	2:A:413:ASN:CB	2.43	0.48
2:A:230:THR:OG1	2:A:232:GLU:OE1	2.31	0.48
2:A:270:LYS:O	2:A:274:ASN:HB2	2.14	0.48
1:B:974:C:H1'	2:A:192:ARG:HB3	1.96	0.48
2:A:151:GLU:H	2:A:151:GLU:CD	2.22	0.48
2:A:455:VAL:HG12	2:A:456:ILE:N	2.28	0.47
2:A:132:TYR:CD2	2:A:141:LYS:HG3	2.50	0.47
2:A:427:GLU:O	2:A:427:GLU:HG2	2.14	0.47
2:A:149:SER:OG	2:A:152:GLU:HG3	2.15	0.47
2:A:367:ASN:HB2	2:A:375:GLY:O	2.14	0.47
2:A:528:SER:HA	2:A:539:ASN:HD21	1.80	0.47
1:B:915:G:P	1:B:916:C:H41	2.38	0.46
1:B:916:C:C5'	1:B:960:U:O2	2.64	0.46
2:A:271:ARG:HD3	2:A:271:ARG:C	2.39	0.46
1:B:976:A:H2''	5:A:996:GLN:CA	2.45	0.46
2:A:369:PRO:O	2:A:371:LYS:N	2.49	0.46
2:A:281:HIS:HE1	6:A:1480:HOH:O	1.99	0.46
2:A:347:ASP:O	2:A:388:ASP:HA	2.16	0.46
2:A:68:THR:CG2	2:A:214:THR:HG21	2.45	0.46
2:A:331:ILE:HG13	2:A:335:LEU:HD22	1.98	0.46
2:A:263:LEU:HB3	2:A:266:THR:HG22	1.98	0.46
2:A:349:VAL:HB	2:A:389:ARG:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:88:LEU:O	2:A:307:ARG:NH1	2.47	0.45
1:B:903:G:O2'	1:B:904:G:H5'	2.16	0.45
2:A:68:THR:HG21	2:A:214:THR:HG21	1.97	0.45
2:A:391:ASP:HA	2:A:402:ARG:HD2	1.98	0.45
2:A:40:HIS:CD2	6:A:1511:HOH:O	2.69	0.45
2:A:114:ILE:HG21	2:A:154:LEU:HD13	1.97	0.45
2:A:533:ALA:HB3	2:A:534:GLU:OE2	2.17	0.45
2:A:40:HIS:HD2	6:A:1511:HOH:O	2.00	0.45
2:A:30:ARG:NH1	2:A:215:HIS:NE2	2.65	0.45
2:A:212:ASP:HB3	2:A:239:LEU:CD2	2.45	0.45
2:A:346:ILE:HG12	2:A:469:ILE:HD13	1.99	0.45
2:A:426:ALA:C	2:A:428:GLY:H	2.25	0.44
2:A:78:VAL:O	2:A:82:LYS:HG3	2.17	0.44
2:A:369:PRO:C	2:A:371:LYS:H	2.25	0.44
2:A:410:ARG:HB3	2:A:455:VAL:HG22	1.99	0.44
2:A:263:LEU:HD22	2:A:324:MET:SD	2.58	0.44
1:B:919:G:O2'	1:B:920:U:C6	2.67	0.44
1:B:934:C:H2'	2:A:412:ARG:HH12	1.83	0.44
2:A:124:LEU:HD12	2:A:128:GLN:HE21	1.78	0.44
2:A:400:TYR:CE2	2:A:402:ARG:HB2	2.53	0.44
2:A:526:LEU:CG	2:A:527:ASP:H	2.15	0.44
2:A:82:LYS:HD2	2:A:96:VAL:HG21	1.99	0.44
2:A:457:HIS:H	2:A:457:HIS:CD2	2.36	0.44
1:B:956:C:H2'	1:B:957:G:O4'	2.18	0.44
2:A:124:LEU:HD22	2:A:143:SER:HB2	2.00	0.44
2:A:527:ASP:C	2:A:529:ARG:N	2.75	0.44
2:A:263:LEU:HB3	2:A:266:THR:CG2	2.48	0.43
2:A:490:VAL:O	2:A:490:VAL:HG13	2.16	0.43
2:A:156:LEU:HD12	2:A:156:LEU:HA	1.82	0.43
2:A:286:ASP:O	2:A:298:ARG:HD3	2.18	0.43
2:A:407:LYS:HG3	2:A:408:GLU:N	2.33	0.43
2:A:442:LEU:N	2:A:442:LEU:CD2	2.80	0.43
1:B:958:A:O2'	1:B:960:U:H5	2.00	0.43
2:A:28:HIS:HE1	2:A:62:ASN:OD1	2.01	0.43
2:A:393:ARG:HB2	2:A:400:TYR:CE2	2.54	0.43
2:A:362:MET:HG3	2:A:378:GLN:HG3	1.99	0.42
4:A:998:AMP:HO3'	5:A:996:GLN:HB2	1.79	0.42
2:A:422:VAL:HG22	2:A:423:GLU:N	2.33	0.42
2:A:487:PHE:O	2:A:490:VAL:HG12	2.18	0.42
2:A:34:GLU:HG3	2:A:66:ASP:O	2.20	0.42
2:A:347:ASP:OD1	2:A:389:ARG:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:403:LEU:HB2	2:A:409:VAL:HG21	2.01	0.42
2:A:313:ILE:CG2	2:A:322:ILE:HG12	2.50	0.42
2:A:410:ARG:HH21	2:A:442:LEU:HA	1.84	0.42
1:B:916:C:H5'	1:B:960:U:O2	2.19	0.42
1:B:958:A:O2'	1:B:959:A:H3'	2.20	0.41
2:A:166:GLU:O	2:A:169:LYS:HB2	2.21	0.41
2:A:343:MET:HE1	2:A:412:ARG:CB	2.45	0.41
1:B:934:C:H1'	2:A:455:VAL:HG21	2.03	0.41
2:A:72:LYS:HE2	2:A:72:LYS:HB3	1.86	0.41
2:A:114:ILE:CG2	2:A:154:LEU:HD13	2.50	0.41
2:A:192:ARG:NE	2:A:194:LYS:HE3	2.35	0.41
2:A:328:GLU:HA	2:A:331:ILE:HG22	2.02	0.41
2:A:519:GLU:HB2	6:A:1493:HOH:O	2.20	0.41
2:A:534:GLU:CD	2:A:534:GLU:N	2.77	0.41
2:A:497:VAL:HG13	2:A:497:VAL:O	2.21	0.41
2:A:229:CYS:O	2:A:257:GLU:HA	2.21	0.40
2:A:269:SER:C	6:A:1511:HOH:O	2.64	0.40
2:A:352:VAL:HG12	2:A:384:GLU:HG2	2.02	0.40
1:B:915:G:H2'	1:B:959:A:N1	2.36	0.40
1:B:919:G:C5	1:B:957:G:N2	2.90	0.40
2:A:151:GLU:CD	2:A:151:GLU:N	2.79	0.40
2:A:391:ASP:OD1	2:A:402:ARG:CD	2.69	0.40
1:B:930:G:HO2'	1:B:931:A:H5'	1.86	0.40
1:B:958:A:HO2'	1:B:960:U:H6	1.62	0.40
2:A:249:ILE:HG13	2:A:250:PRO:HD2	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	525/553 (95%)	496 (94%)	19 (4%)	10 (2%)	6 11

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	32	PRO
2	A	370	ASN
2	A	397	ASN
2	A	405	LEU
2	A	526	LEU
2	A	527	ASP
2	A	369	PRO
2	A	396	ALA
2	A	426	ALA
2	A	176	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	463/481 (96%)	430 (93%)	33 (7%)	13	29

All (33) 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	49	LEU
2	A	78	VAL
2	A	82	LYS
2	A	105	GLN
2	A	106	LEU
2	A	124	LEU
2	A	148	ARG
2	A	154	LEU
2	A	156	LEU
2	A	159	LYS
2	A	173	ARG

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Mol	Chain	Res	Type
2	A	186	ARG
2	A	190	LEU
2	A	192	ARG
2	A	231	LEU
2	A	232	GLU
2	A	263	LEU
2	A	270	LYS
2	A	327	LEU
2	A	335	LEU
2	A	341	ARG
2	A	395	GLU
2	A	398	LYS
2	A	408	GLU
2	A	412	ARG
2	A	441	THR
2	A	475	LEU
2	A	490	VAL
2	A	544	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	28	HIS
2	A	55	GLN
2	A	95	ASN
2	A	115	ASN
2	A	128	GLN
2	A	138	GLN
2	A	142	ASN
2	A	153	ASN
2	A	226	HIS
2	A	236	ASN
2	A	281	HIS
2	A	429	ASN
2	A	457	HIS
2	A	480	ASN
2	A	530	HIS
2	A	539	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	72/75 (96%)	19 (26%)	7 (9%)

All (19) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	908	U
1	B	909	C
1	B	910	G
1	B	916	C
1	B	918	G
1	B	920	U
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	945	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

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	907	A
1	B	916	C
1	B	919	G
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 ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	1394	-	4,4,4	0.41	0	6,6,6	0.09	0
3	SO4	A	1395	-	4,4,4	0.34	0	6,6,6	0.14	0
4	AMP	A	998	-	25,25,25	0.38	0	37,38,38	0.48	0
5	GLN	A	996	-	8,9,9	0.79	0	8,11,11	0.50	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
4	AMP	A	998	-	-	3/10/26/26	0/3/3/3
5	GLN	A	996	-	-	4/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	996	GLN	O-C-CA-N
5	A	996	GLN	OXT-C-CA-N
4	A	998	AMP	C5'-O5'-P-O2P
4	A	998	AMP	C5'-O5'-P-O1P

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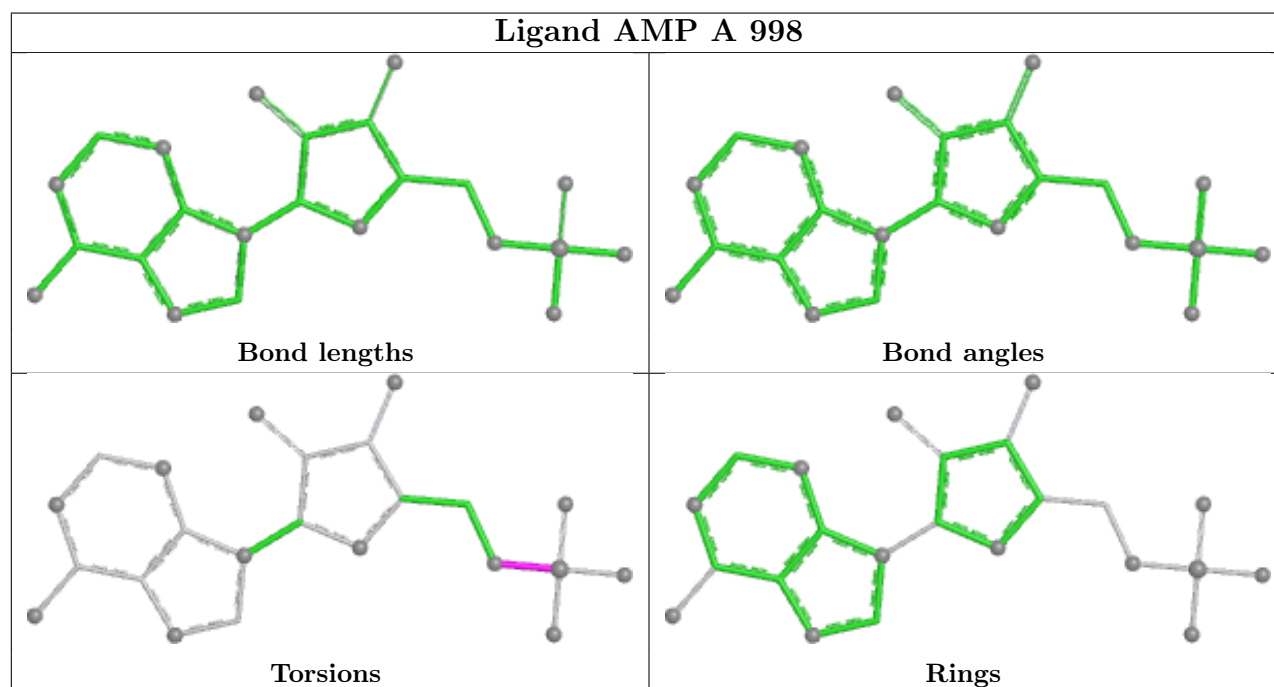
Mol	Chain	Res	Type	Atoms
4	A	998	AMP	C5'-O5'-P-O3P
5	A	996	GLN	O-C-CA-CB
5	A	996	GLN	OXT-C-CA-CB

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	998	AMP	3	0
5	A	996	GLN	7	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

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	74/75 (98%)	1.51	27 (36%) 1 1	32, 77, 130, 171	0
2	A	529/553 (95%)	0.35	52 (9%) 13 11	16, 34, 81, 112	0
All	All	603/628 (96%)	0.49	79 (13%) 7 6	16, 37, 95, 171	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	442	LEU	8.0
2	A	547	THR	7.2
2	A	439	ALA	7.1
2	A	426	ALA	6.0
1	B	920	U	5.7
2	A	513	GLY	5.7
1	B	947	U	5.7
2	A	528	SER	5.0
2	A	529	ARG	4.8
2	A	398	LYS	4.7
2	A	440	ASP	4.4
2	A	408	GLU	4.3
2	A	527	ASP	4.3
2	A	405	LEU	4.2
2	A	533	ALA	4.2
1	B	934	C	4.1
1	B	946	U	4.1
1	B	958	A	4.1
2	A	355	ASN	4.0
2	A	427	GLU	4.0
1	B	945	A	4.0
1	B	919	G	3.9
2	A	407	LYS	3.9
2	A	357	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
2	A	419	ALA	3.8
1	B	909	C	3.7
2	A	534	GLU	3.7
1	B	948	C	3.6
1	B	921	A	3.6
2	A	421	ARG	3.5
2	A	395	GLU	3.4
1	B	956	C	3.4
2	A	441	THR	3.3
1	B	916	C	3.2
1	B	941	C	3.1
2	A	511	VAL	3.1
2	A	393	ARG	2.9
2	A	422	VAL	2.8
2	A	318	GLN	2.8
1	B	955	U	2.8
1	B	936	G	2.8
2	A	545	ARG	2.7
2	A	454	GLY	2.7
1	B	918	G	2.7
2	A	414	ALA	2.6
1	B	929	G	2.6
1	B	957	G	2.6
2	A	409	VAL	2.6
1	B	952	G	2.5
2	A	401	LYS	2.5
2	A	420	GLU	2.5
2	A	72	LYS	2.5
2	A	400	TYR	2.5
2	A	396	ALA	2.5
1	B	959	A	2.4
1	B	944	C	2.4
1	B	933	U	2.4
1	B	954	U	2.4
2	A	399	GLN	2.4
2	A	369	PRO	2.3
1	B	931	A	2.3
2	A	535	LYS	2.3
2	A	271	ARG	2.3
2	A	532	THR	2.3
2	A	428	GLY	2.3
2	A	431	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	960	U	2.2
2	A	354	GLU	2.2
2	A	509	ASP	2.2
2	A	435	CYS	2.2
2	A	406	GLY	2.2
2	A	425	ASP	2.2
1	B	932	U	2.2
2	A	138	GLN	2.2
2	A	432	THR	2.1
2	A	418	LYS	2.1
2	A	58	LYS	2.1
2	A	508	LYS	2.0
1	B	915	G	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](#)

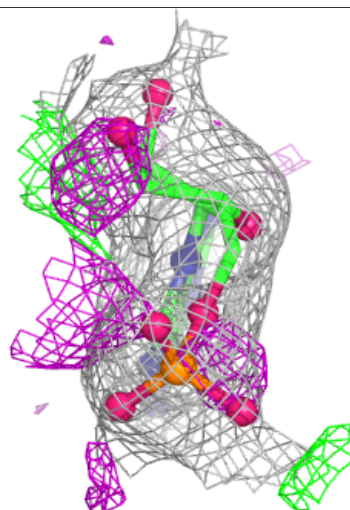
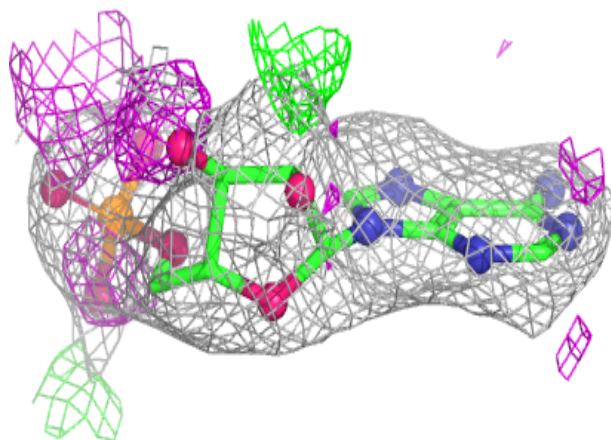
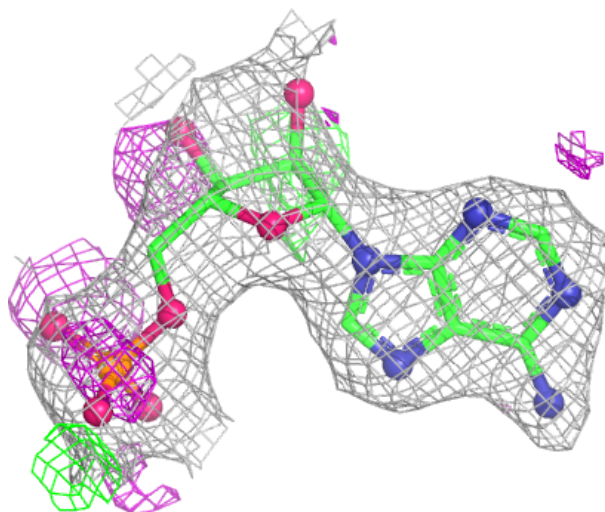
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GLN	A	996	10/10	0.82	0.22	51,58,64,80	0
4	AMP	A	998	23/23	0.90	0.13	29,47,58,60	0
3	SO4	A	1394	5/5	0.92	0.21	81,81,88,89	0
3	SO4	A	1395	5/5	0.93	0.12	67,68,70,72	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.

Electron density around AMP A 998:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.