



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:08 AM UTC

PDB ID : 1O0B / pdb_00001o0b
Title : CRYSTAL STRUCTURE OF L-GLUTAMINE 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 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

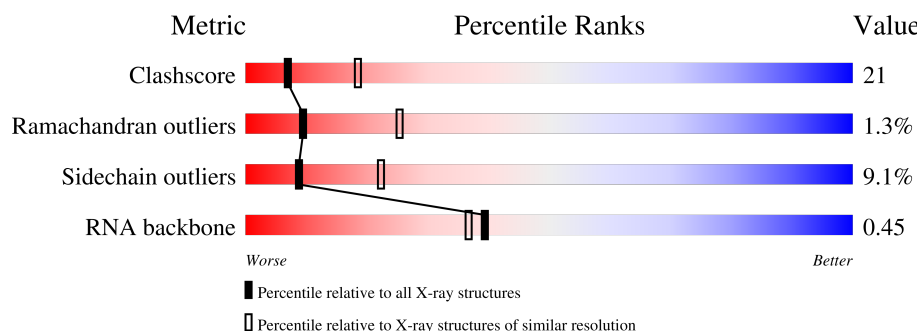
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

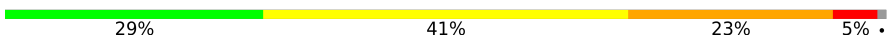
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

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	

2 Entry composition

There are 6 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 Glutaminyl tRNA.

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

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
2	A	529	Total	C	N	O	S	0	0	0
			4279	2704	752	802	21			

There is a discrepancy between the modelled and reference sequences:

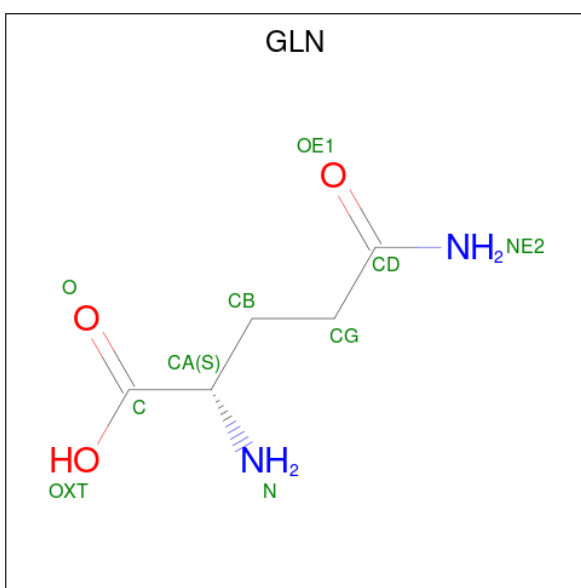
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	cloning artifact	UNP P00962

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



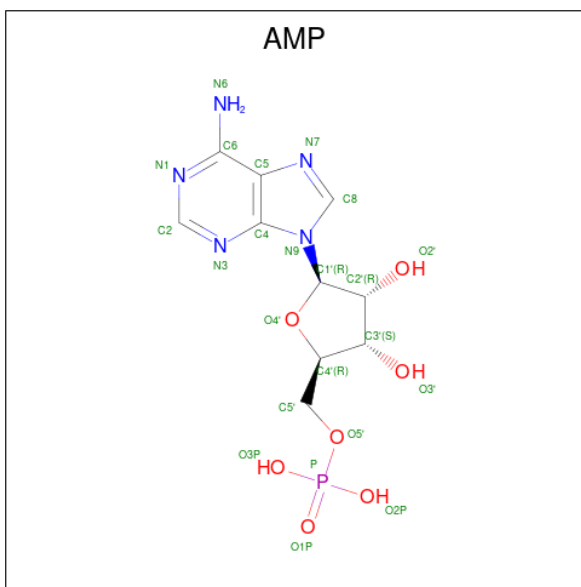
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLUTAMINE (CCD ID: GLN) (formula: $C_5H_{10}N_2O_3$).



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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			19	10	5	4		

- Molecule 6 is water.

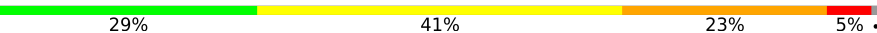
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	28	Total	O	0	0
			28	28		
6	A	116	Total	O	0	0
			116	116		

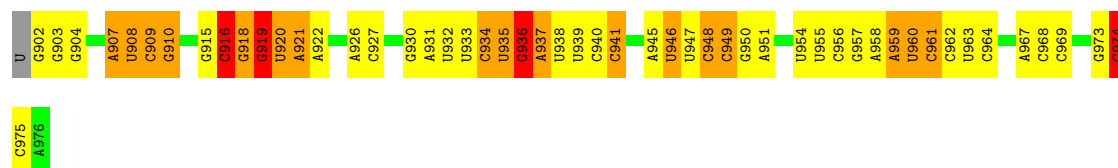
3 Residue-property plots

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.

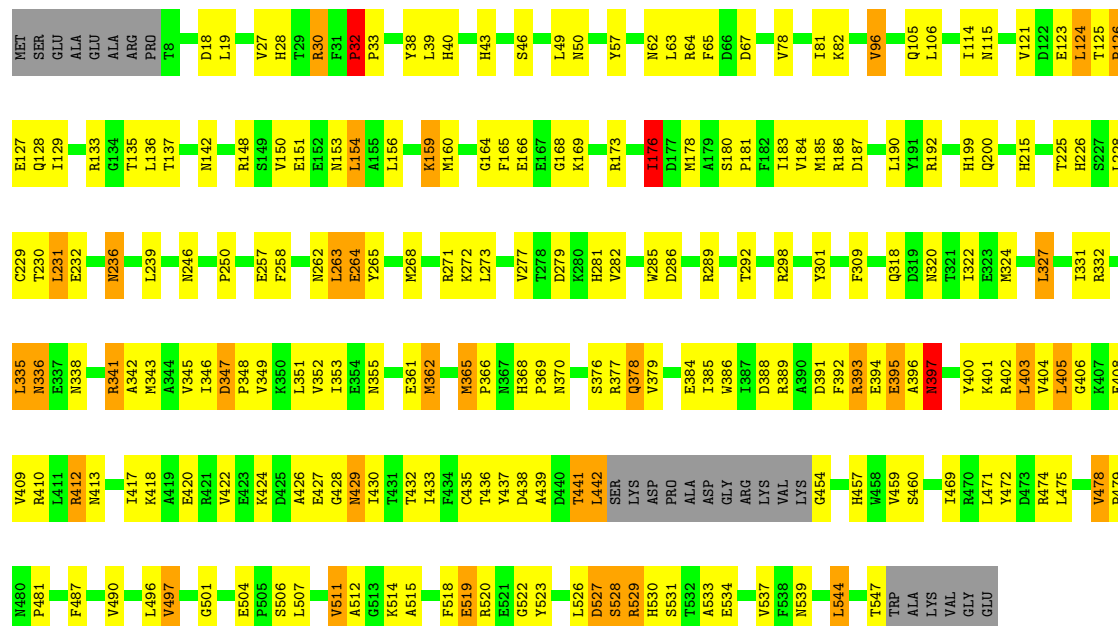
• Molecule 1: Glutaminyl tRNA

Chain B: 



• Molecule 2: Glutaminyl-tRNA synthetase

Chain A: 



4 Data and refinement statistics

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	236.45Å 92.89Å 114.71Å 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}	0.04	Depositor
R_{sym}	0.03	Depositor
Refinement program	X-PLOR 98.1	Depositor
R, R_{free}	0.216 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6032	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

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	0.45	0/1753	0.87	7/2730 (0.3%)
2	A	0.55	0/4379	1.02	22/5928 (0.4%)
All	All	0.52	0/6132	0.97	29/8658 (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	3

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	338	ASN	N-CA-C	7.83	122.97	113.41
2	A	215	HIS	N-CA-C	7.80	120.47	111.11
2	A	32	PRO	N-CA-C	7.53	119.89	110.70
2	A	478	VAL	CA-C-N	7.41	127.43	119.28
2	A	478	VAL	C-N-CA	7.41	127.43	119.28
2	A	67	ASP	N-CA-C	7.07	119.68	109.71
2	A	231	LEU	N-CA-C	7.07	120.80	111.75
1	B	919	G	N9-C1'-C2'	6.99	122.48	112.00
2	A	403	LEU	N-CA-C	6.73	119.49	109.59
2	A	365	MET	CA-C-N	6.44	126.40	119.76
2	A	365	MET	C-N-CA	6.44	126.40	119.76
2	A	250	PRO	N-CA-C	6.41	121.88	113.86
1	B	974	C	C4'-C3'-O3'	-6.28	99.98	109.40
1	B	916	C	C2'-C3'-O3'	5.85	118.27	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	936	G	N9-C1'-C2'	5.77	122.66	114.00
2	A	181	PRO	N-CA-C	-5.63	106.82	113.86
2	A	518	PHE	N-CA-C	-5.51	100.13	108.67
1	B	945	A	N9-C1'-C2'	5.47	120.20	112.00
1	B	974	C	N1-C1'-C2'	5.42	122.13	114.00
2	A	246	ASN	N-CA-C	5.40	119.85	112.88
2	A	133	ARG	N-CA-C	5.22	117.71	111.71
2	A	63	LEU	N-CA-C	-5.21	100.03	108.52
2	A	347	ASP	CA-C-N	-5.21	113.33	119.84
2	A	347	ASP	C-N-CA	-5.21	113.33	119.84
1	B	919	G	C4'-C3'-O3'	-5.12	105.32	113.00
2	A	348	PRO	N-CA-C	5.10	122.97	112.47
2	A	142	ASN	N-CA-C	5.05	117.55	110.23
2	A	96	VAL	N-CA-C	-5.04	102.24	108.89
2	A	50	ASN	N-CA-C	5.03	116.57	111.14

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	919	G	Sidechain
1	B	936	G	Sidechain
1	B	948	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	1570	0	801	77	0
2	A	4279	0	4172	162	0
3	A	10	0	0	1	0
4	A	10	0	7	1	0
5	A	19	0	12	6	0
6	A	116	0	0	5	0
6	B	28	0	0	0	0
All	All	6032	0	4992	225	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 21.

All (225) 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:C5	1.84	1.13
1:B:946:U:H4'	1:B:947:U:C6	1.91	1.06
2:A:526:LEU:HG	2:A:527:ASP:H	1.35	0.92
2:A:522:GLY:HA2	2:A:544:LEU:HD13	1.51	0.90
1:B:918:G:H4'	1:B:919:G:OP1	1.73	0.88
1:B:963:U:H2'	1:B:964:C:C6	2.09	0.88
2:A:410:ARG:HH21	2:A:442:LEU:HA	1.40	0.86
1:B:915:G:H2'	1:B:959:A:N1	1.91	0.85
2:A:39:LEU:HD13	2:A:81:ILE:HG12	1.59	0.85
1:B:930:G:O2'	1:B:931:A:H5'	1.78	0.84
1:B:921:A:H62	1:B:947:U:H1'	1.45	0.82
1:B:947:U:H2'	1:B:947:U:O2	1.81	0.81
2:A:352:VAL:HG12	2:A:384:GLU:HG2	1.67	0.75
2:A:531:SER:HB3	2:A:537:VAL:H	1.51	0.75
1:B:960:U:H5'	1:B:961:C:OP2	1.89	0.72
1:B:946:U:C4'	1:B:947:U:C5	2.70	0.72
2:A:471:LEU:HB2	2:A:497:VAL:HG13	1.73	0.70
2:A:82:LYS:HD3	2:A:96:VAL:HG21	1.74	0.69
1:B:934:C:H4'	1:B:935:U:OP1	1.90	0.69
2:A:39:LEU:CD1	2:A:81:ILE:HG12	2.24	0.68
2:A:403:LEU:HD13	2:A:409:VAL:HG22	1.75	0.68
2:A:125:THR:HG23	2:A:128:GLN:NE2	2.08	0.68
2:A:341:ARG:HD3	2:A:369:PRO:HD2	1.77	0.66
1:B:962:C:O2'	1:B:963:U:H5'	1.96	0.66
2:A:410:ARG:NH2	2:A:442:LEU:HA	2.11	0.66
2:A:124:LEU:HG	2:A:128:GLN:HB3	1.77	0.66
1:B:918:G:C4'	1:B:919:G:OP1	2.44	0.66
2:A:264:GLU:O	2:A:324:MET:HE2	1.96	0.66
1:B:939:U:O2'	1:B:940:C:H5'	1.97	0.64
2:A:393:ARG:O	2:A:404:VAL:HA	1.97	0.64
2:A:28:HIS:HE1	2:A:62:ASN:OD1	1.80	0.64
1:B:903:G:O2'	1:B:904:G:H5'	1.97	0.63
1:B:916:C:OP2	1:B:916:C:H3'	1.98	0.63
1:B:921:A:N6	1:B:947:U:H1'	2.14	0.62
1:B:955:U:H2'	1:B:957:G:OP2	1.98	0.62
2:A:474:ARG:HD2	6:A:1489:HOH:O	1.99	0.62
2:A:272:LYS:HD2	3:A:1395:SO4:O1	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:511:VAL:HG23	2:A:514:LYS:HB3	1.83	0.61
2:A:457:HIS:HD2	2:A:520:ARG:HE	1.48	0.61
2:A:427:GLU:HB3	2:A:429:ASN:OD1	2.01	0.60
2:A:438:ASP:HB3	2:A:441:THR:OG1	2.00	0.60
1:B:916:C:H5''	1:B:960:U:O2	2.00	0.60
2:A:30:ARG:NH2	2:A:228:LEU:O	2.35	0.60
2:A:115:ASN:HD21	2:A:154:LEU:HD21	1.66	0.60
2:A:114:ILE:HG21	2:A:154:LEU:HD13	1.84	0.60
1:B:954:U:H2'	1:B:955:U:C6	2.37	0.60
1:B:960:U:H5''	1:B:961:C:H5	1.67	0.59
2:A:362:MET:CG	2:A:378:GLN:HG3	2.33	0.59
2:A:335:LEU:HB3	2:A:523:TYR:CD1	2.39	0.58
2:A:114:ILE:CG2	2:A:154:LEU:HD13	2.33	0.58
2:A:341:ARG:HB3	6:A:1494:HOH:O	2.02	0.58
2:A:512:ALA:HB1	2:A:527:ASP:HB2	1.85	0.58
1:B:958:A:HO2'	1:B:960:U:H5	1.47	0.57
1:B:935:U:O2'	2:A:520:ARG:HG2	2.05	0.57
2:A:40:HIS:HA	2:A:292:THR:HA	1.86	0.57
1:B:950:G:H2'	1:B:951:A:C8	2.40	0.57
2:A:236:ASN:H	2:A:236:ASN:HD22	1.51	0.57
2:A:43:HIS:HD2	5:A:998:AMP:O4'	1.89	0.56
2:A:166:GLU:O	2:A:169:LYS:HB2	2.05	0.56
2:A:335:LEU:HD23	2:A:523:TYR:CB	2.36	0.56
2:A:301:TYR:HE2	2:A:327:LEU:HD22	1.70	0.56
2:A:424:LYS:HA	2:A:430:ILE:HA	1.88	0.55
2:A:424:LYS:HD3	2:A:428:GLY:O	2.06	0.55
2:A:343:MET:HE1	2:A:412:ARG:HB3	1.89	0.55
2:A:281:HIS:HE1	6:A:1480:HOH:O	1.89	0.55
1:B:918:G:H5''	1:B:919:G:OP1	2.07	0.55
2:A:46:SER:HB2	5:A:998:AMP:H1'	1.89	0.54
2:A:173:ARG:HD2	2:A:187:ASP:O	2.07	0.54
2:A:273:LEU:O	2:A:277:VAL:HG23	2.08	0.54
1:B:958:A:O2'	1:B:960:U:C5	2.57	0.54
2:A:159:LYS:HD3	2:A:164:GLY:HA3	1.90	0.54
2:A:519:GLU:HB2	6:A:1494:HOH:O	2.06	0.54
1:B:921:A:N6	1:B:947:U:O2'	2.40	0.54
2:A:422:VAL:HG21	2:A:430:ILE:HD13	1.90	0.54
1:B:934:C:HO2'	2:A:412:ARG:HH22	1.57	0.53
1:B:908:U:H5'	1:B:949:C:OP2	2.09	0.53
2:A:487:PHE:O	2:A:490:VAL:HG12	2.09	0.53
2:A:353:ILE:HG21	2:A:437:TYR:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:937:A:H2'	1:B:938:U:O4'	2.09	0.53
2:A:362:MET:HG2	2:A:378:GLN:HG3	1.91	0.53
1:B:940:C:H2'	1:B:941:C:C6	2.44	0.53
1:B:947:U:O2	1:B:947:U:C2'	2.51	0.52
2:A:393:ARG:HB2	2:A:400:TYR:CE2	2.43	0.52
1:B:931:A:H2'	1:B:932:U:O4'	2.09	0.52
1:B:934:C:O2'	2:A:412:ARG:NH1	2.43	0.52
2:A:265:TYR:CD1	2:A:474:ARG:HD3	2.44	0.52
2:A:289:ARG:HE	2:A:496:LEU:HB2	1.73	0.52
2:A:32:PRO:HA	2:A:64:ARG:O	2.09	0.52
1:B:903:G:C2'	1:B:904:G:H5'	2.40	0.51
2:A:355:ASN:HB2	2:A:436:THR:HA	1.92	0.51
2:A:301:TYR:CE2	2:A:327:LEU:HD22	2.45	0.51
2:A:526:LEU:CG	2:A:527:ASP:H	2.15	0.51
2:A:346:ILE:N	2:A:346:ILE:HD12	2.25	0.51
1:B:916:C:H2'	1:B:916:C:O2	2.10	0.51
2:A:386:TRP:N	2:A:459:VAL:O	2.44	0.51
2:A:126:PRO:O	2:A:129:ILE:HG22	2.11	0.50
1:B:956:C:H2'	1:B:957:G:O4'	2.10	0.50
1:B:932:U:C4	1:B:933:U:C4	3.00	0.50
1:B:961:C:C2	1:B:962:C:C5	3.00	0.50
1:B:916:C:O2	1:B:916:C:C2'	2.58	0.50
2:A:18:ASP:OD2	2:A:226:HIS:HE1	1.95	0.50
2:A:397:ASN:ND2	2:A:400:TYR:HB2	2.27	0.50
5:A:998:AMP:H2'	6:A:1492:HOH:O	2.12	0.50
2:A:388:ASP:HB3	2:A:391:ASP:OD2	2.11	0.50
1:B:955:U:H6	1:B:955:U:O5'	1.93	0.49
1:B:958:A:HO2'	1:B:960:U:H6	1.48	0.49
2:A:528:SER:O	2:A:530:HIS:CD2	2.65	0.49
1:B:974:C:N3	2:A:168:GLY:HA2	2.27	0.49
2:A:472:TYR:HE2	2:A:539:ASN:OD1	1.96	0.49
1:B:902:G:C8	2:A:137:THR:HG22	2.48	0.49
1:B:936:G:OP2	2:A:401:LYS:NZ	2.45	0.49
2:A:526:LEU:HG	2:A:527:ASP:N	2.17	0.49
2:A:150:VAL:HG12	2:A:154:LEU:HD22	1.95	0.48
2:A:229:CYS:SG	2:A:257:GLU:HG3	2.52	0.48
1:B:934:C:O2'	2:A:412:ARG:NH2	2.46	0.48
2:A:286:ASP:O	2:A:298:ARG:HD3	2.13	0.48
1:B:915:G:C2'	1:B:959:A:N1	2.72	0.48
2:A:282:VAL:HG12	2:A:289:ARG:NH1	2.27	0.48
2:A:514:LYS:HG2	2:A:515:ALA:N	2.28	0.48

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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	0.48
2:A:418:LYS:HD2	2:A:420:GLU:OE2	2.13	0.48
4:A:996:GLN:OXT	5:A:998:AMP:H5'2	2.13	0.48
1:B:903:G:HO2'	1:B:904:G:H5'	1.80	0.47
1:B:954:U:H2'	1:B:955:U:H6	1.77	0.47
2:A:262:ASN:HB2	2:A:320:ASN:O	2.13	0.47
1:B:919:G:O2'	1:B:920:U:C6	2.68	0.47
2:A:335:LEU:HD23	2:A:523:TYR:HB3	1.95	0.47
2:A:393:ARG:HB2	2:A:400:TYR:CZ	2.50	0.47
1:B:907:A:C2	1:B:967:A:C2	3.02	0.47
1:B:958:A:O2'	1:B:960:U:H5	1.94	0.47
2:A:136:LEU:HD23	2:A:183:ILE:CD1	2.44	0.47
2:A:401:LYS:HE2	2:A:454:GLY:HA3	1.97	0.47
2:A:422:VAL:HG23	2:A:433:ILE:HG13	1.97	0.47
2:A:365:MET:HG2	2:A:413:ASN:CB	2.45	0.47
1:B:926:A:C2'	1:B:927:C:H5'	2.45	0.47
1:B:936:G:C2	2:A:401:LYS:HG2	2.49	0.47
1:B:958:A:O2'	1:B:959:A:H3'	2.14	0.47
2:A:349:VAL:HB	2:A:389:ARG:HG2	1.96	0.47
2:A:394:GLU:HA	2:A:405:LEU:HB2	1.97	0.47
2:A:335:LEU:HB3	2:A:523:TYR:CE1	2.50	0.46
1:B:961:C:H2'	1:B:962:C:H6	1.81	0.46
2:A:271:ARG:HD3	2:A:271:ARG:C	2.39	0.46
2:A:392:PHE:HA	2:A:403:LEU:O	2.15	0.46
2:A:33:PRO:HA	5:A:998:AMP:H5'2	1.97	0.46
1:B:926:A:O2'	1:B:927:C:H5'	2.16	0.46
2:A:121:VAL:H	2:A:153:ASN:ND2	2.14	0.46
2:A:346:ILE:HG13	2:A:469:ILE:HD13	1.96	0.46
2:A:127:GLU:CD	2:A:127:GLU:N	2.74	0.46
2:A:365:MET:HE3	2:A:379:VAL:HB	1.97	0.46
2:A:408:GLU:HA	2:A:417:ILE:O	2.15	0.46
2:A:65:PHE:HE2	2:A:96:VAL:HG11	1.80	0.45
1:B:935:U:O2	2:A:519:GLU:HG3	2.16	0.45
1:B:907:A:H5'	2:A:318:GLN:NE2	2.32	0.45
2:A:533:ALA:HB3	2:A:534:GLU:OE2	2.17	0.45
2:A:151:GLU:H	2:A:151:GLU:CD	2.25	0.45
2:A:159:LYS:HD2	2:A:165:PHE:CE2	2.52	0.45
2:A:365:MET:HG2	2:A:413:ASN:OD1	2.16	0.45
2:A:504:GLU:HG3	2:A:506:SER:HB3	1.99	0.45
2:A:46:SER:CB	5:A:998:AMP:H1'	2.47	0.45
2:A:159:LYS:HD2	2:A:165:PHE:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:385:ILE:HA	2:A:460:SER:HA	1.99	0.45
2:A:393:ARG:HG2	2:A:396:ALA:CB	2.47	0.44
2:A:38:TYR:HB2	2:A:285:TRP:CE3	2.53	0.44
1:B:916:C:C5'	1:B:960:U:O2	2.65	0.44
1:B:918:G:C5'	1:B:919:G:OP1	2.64	0.44
2:A:279:ASP:HB3	2:A:281:HIS:CE1	2.52	0.44
2:A:527:ASP:CG	2:A:529:ARG:H	2.26	0.44
1:B:937:A:C2	1:B:938:U:H1'	2.53	0.44
1:B:968:C:H2'	1:B:969:C:H6	1.81	0.44
2:A:391:ASP:OD1	2:A:402:ARG:HD2	2.18	0.44
1:B:902:G:C4	2:A:136:LEU:O	2.71	0.44
1:B:936:G:C4	2:A:401:LYS:HD3	2.52	0.44
2:A:522:GLY:CA	2:A:544:LEU:HD13	2.36	0.44
1:B:956:C:H6	1:B:956:C:O5'	2.00	0.44
1:B:936:G:N1	2:A:401:LYS:HG2	2.33	0.43
2:A:478:VAL:HA	2:A:479:PRO:HD3	1.87	0.43
2:A:135:THR:O	2:A:186:ARG:NH2	2.50	0.43
1:B:907:A:C5'	2:A:318:GLN:NE2	2.82	0.43
2:A:343:MET:HE1	2:A:412:ARG:CB	2.48	0.43
2:A:427:GLU:O	2:A:427:GLU:HG2	2.19	0.43
2:A:230:THR:HA	2:A:258:PHE:O	2.18	0.43
1:B:934:C:C4'	1:B:935:U:OP1	2.64	0.43
2:A:309:PHE:CE1	2:A:322:ILE:HG21	2.54	0.43
2:A:183:ILE:HA	2:A:186:ARG:HG3	2.00	0.42
2:A:335:LEU:HD23	2:A:523:TYR:CG	2.54	0.42
2:A:176:ILE:HB	2:A:185:MET:O	2.20	0.42
2:A:124:LEU:HD12	2:A:128:GLN:OE1	2.20	0.42
1:B:903:G:H2'	1:B:904:G:O4'	2.20	0.42
1:B:909:C:H5''	1:B:910:G:OP2	2.20	0.42
1:B:955:U:C2'	1:B:957:G:OP2	2.66	0.42
2:A:123:GLU:HG3	2:A:148:ARG:NH2	2.35	0.42
2:A:199:HIS:ND1	2:A:200:GLN:HG2	2.35	0.42
2:A:368:HIS:HD2	2:A:370:ASN:H	1.67	0.42
2:A:442:LEU:N	2:A:442:LEU:HD23	2.34	0.42
2:A:362:MET:HG3	2:A:378:GLN:HG3	2.02	0.41
2:A:366:PRO:HA	2:A:376:SER:OG	2.20	0.41
2:A:426:ALA:C	2:A:428:GLY:H	2.28	0.41
1:B:916:C:O2'	1:B:918:G:P	2.77	0.41
2:A:347:ASP:O	2:A:388:ASP:HA	2.19	0.41
2:A:27:VAL:HG21	2:A:57:TYR:HB2	2.02	0.41
2:A:343:MET:CE	2:A:412:ARG:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:393:ARG:HG2	2:A:396:ALA:HB2	2.01	0.41
2:A:225:THR:OG1	2:A:226:HIS:HD2	2.03	0.41
2:A:351:LEU:HG	2:A:435:CYS:SG	2.61	0.41
2:A:433:ILE:HG22	2:A:435:CYS:SG	2.61	0.41
1:B:902:G:C8	2:A:137:THR:CG2	3.04	0.41
1:B:930:G:C2'	1:B:931:A:H5'	2.50	0.41
1:B:960:U:H5''	1:B:961:C:C5	2.50	0.41
2:A:160:MET:HE2	2:A:160:MET:HB3	1.98	0.41
2:A:184:VAL:HG22	2:A:239:LEU:HD22	2.03	0.41
2:A:351:LEU:C	2:A:351:LEU:HD23	2.46	0.41
2:A:478:VAL:O	2:A:481:PRO:HD3	2.21	0.41
2:A:18:ASP:OD2	2:A:226:HIS:CE1	2.73	0.41
2:A:332:ARG:O	2:A:336:ASN:HB3	2.20	0.41
2:A:346:ILE:HG13	2:A:469:ILE:CD1	2.50	0.41
2:A:527:ASP:HA	2:A:531:SER:OG	2.22	0.41
2:A:331:ILE:HG13	2:A:335:LEU:HD22	2.03	0.40
2:A:178:MET:O	2:A:186:ARG:HD2	2.21	0.40
2:A:263:LEU:HB2	2:A:268:MET:CE	2.51	0.40
2:A:361:GLU:HG3	2:A:362:MET:N	2.36	0.40
2:A:395:GLU:CD	2:A:395:GLU:N	2.78	0.40
2:A:342:ALA:HB1	2:A:507:LEU:HD21	2.03	0.40
1:B:935:U:O3'	2:A:520:ARG:HD2	2.22	0.40
2:A:345:VAL:O	2:A:501:GLY:HA3	2.20	0.40
2:A:377:ARG:HH11	2:A:377:ARG:HG2	1.86	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%)	492 (94%)	26 (5%)	7 (1%)	9	25

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	397	ASN
2	A	32	PRO
2	A	405	LEU
2	A	527	ASP
2	A	406	GLY
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%)	421 (91%)	42 (9%)	9 22

All (42) 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	49	LEU
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	176	ILE
2	A	190	LEU
2	A	192	ARG
2	A	231	LEU
2	A	232	GLU
2	A	236	ASN

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Mol	Chain	Res	Type
2	A	263	LEU
2	A	264	GLU
2	A	327	LEU
2	A	335	LEU
2	A	336	ASN
2	A	341	ARG
2	A	362	MET
2	A	378	GLN
2	A	393	ARG
2	A	395	GLU
2	A	397	ASN
2	A	412	ARG
2	A	429	ASN
2	A	432	THR
2	A	441	THR
2	A	442	LEU
2	A	475	LEU
2	A	497	VAL
2	A	511	VAL
2	A	519	GLU
2	A	528	SER
2	A	529	ARG
2	A	544	LEU
2	A	547	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) 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	281	HIS
2	A	318	GLN
2	A	320	ASN
2	A	368	HIS
2	A	378	GLN
2	A	397	ASN
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%)	11 (15%)

All (21) 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	919	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	946	U
1	B	948	C
1	B	949	C
1	B	959	A
1	B	961	C
1	B	973	G
1	B	974	C
1	B	975	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	C
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](#)

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	$\# Z > 2$
4	GLN	A	996	-	8,9,9	0.99	0	8,11,11	0.15	0
5	AMP	A	998	-	21,21,25	0.28	0	31,31,38	0.35	0
3	SO4	A	1394	-	4,4,4	0.73	0	6,6,6	0.38	0
3	SO4	A	1395	-	4,4,4	0.80	0	6,6,6	0.49	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	GLN	A	996	-	-	0/9/9/9	-
5	AMP	A	998	-	-	0/6/22/26	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	996	GLN	1	0
5	A	998	AMP	6	0
3	A	1395	SO4	1	0

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.