



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:17 PM GMT

PDB ID : 1EXD  
Title : CRYSTAL STRUCTURE OF A TIGHT-BINDING GLUTAMINE TRNA  
BOUND TO GLUTAMINE AMINOACYL TRNA SYNTHETASE  
Authors : Bullock, T.L.; Sherlin, L.D.; Perona, J.J.  
Deposited on : 2000-05-02  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

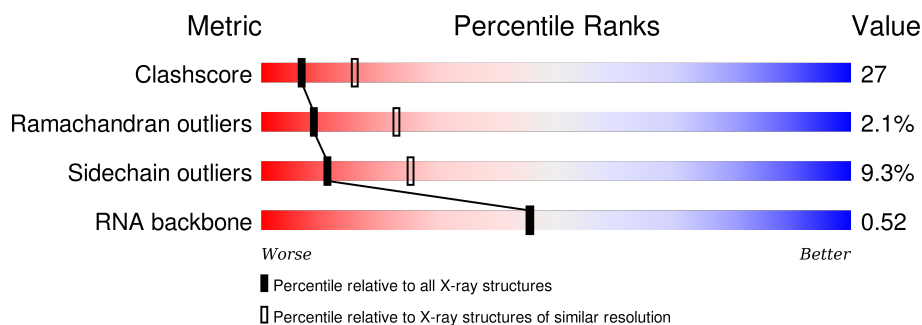
# 1 Overall quality at a glance

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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RNA backbone	2183	1069 (3.10-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	73	
2	A	548	

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
3	SO4	A	1395	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6031 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.

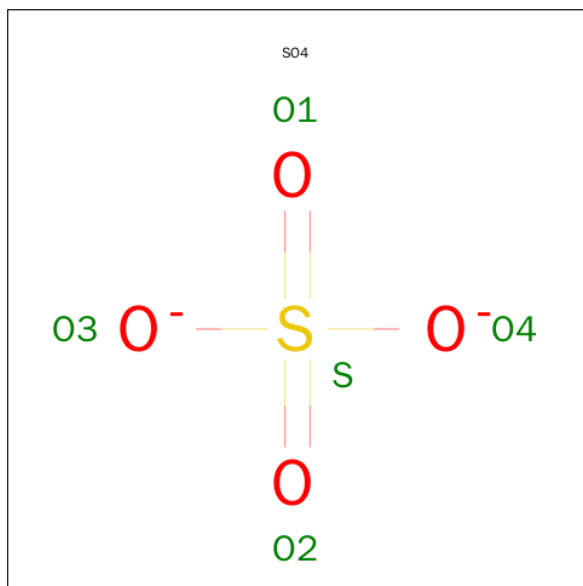
- Molecule 1 is a RNA chain called GLUTAMINE TRNA APTAMER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	73	Total	C	N	O	P	0	0	0
			1556	695	281	508	72			

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

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

- Molecule 3 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



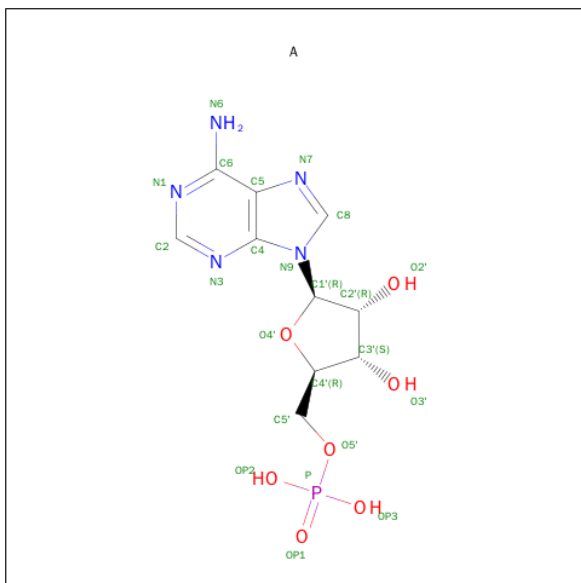
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 4 is ADENOSINE-5'-MONOPHOSPHATE (three-letter code: A) (formula:  $C_{10}H_{14}N_5O_7P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	122	Total	O	0	0
			122	122		
5	B	37	Total	O	0	0
			37	37		

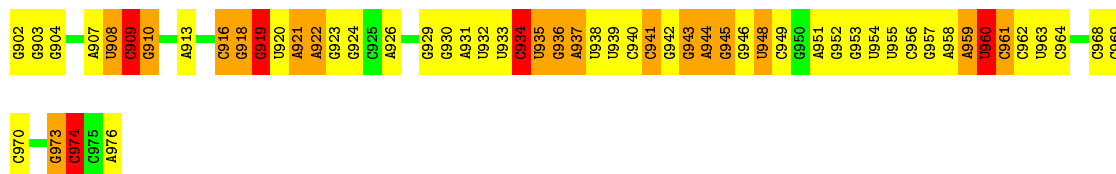
### 3 Residue-property plots

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

Note EDS was not executed.

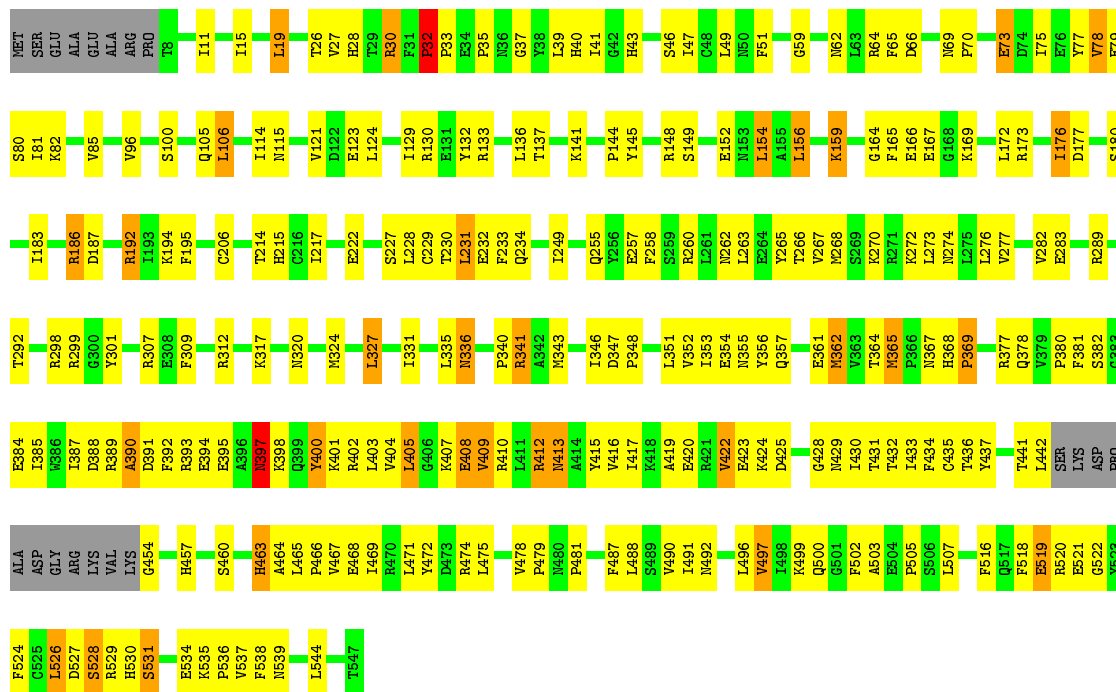
#### • Molecule 1: GLUTAMINE TRNA APTAMER

Chain B: 



#### • Molecule 2: GLUTAMINYL-TRNA SYNTHETASE

Chain A: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	236.94Å 93.98Å 113.91Å 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
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 98.0	Depositor
R, $R_{free}$	0.216 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6031	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	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

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	0.56	0/1739	0.89	7/2710 (0.3%)
2	A	0.47	0/4379	0.70	1/5928 (0.0%)
All	All	0.50	0/6118	0.77	8/8638 (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	3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	974	C	N1-C1'-C2'	6.87	122.93	114.00
1	B	919	G	N9-C1'-C2'	6.47	122.41	114.00
1	B	936	G	N9-C1'-C2'	6.44	122.37	114.00
1	B	960	U	N1-C1'-C2'	6.33	122.22	114.00
1	B	934	C	N1-C1'-C2'	6.14	121.98	114.00
2	A	397	ASN	N-CA-C	5.44	125.69	111.00
1	B	909	C	C4'-C3'-O3'	-5.25	98.37	109.40
1	B	909	C	N1-C1'-C2'	5.01	120.51	114.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	919	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	1556	0	791	99	0
2	A	4279	0	4172	201	0
3	A	10	0	0	3	0
3	B	5	0	0	0	0
4	A	22	0	12	5	0
5	A	122	0	0	4	0
5	B	37	0	0	0	0
All	All	6031	0	4975	288	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 27.

All (288) 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:919:G:H1'	1:B:920:U:C5	1.84	1.12
2:A:362:MET:HG2	2:A:378:GLN:HG3	1.24	1.11
1:B:918:G:H4'	1:B:919:G:OP1	1.56	1.04
1:B:919:G:H1'	1:B:920:U:H5	1.19	1.04
1:B:921:A:H61	1:B:946:G:H2'	1.22	1.00
1:B:939:U:H2'	1:B:940:C:H6	1.22	1.00
2:A:353:ILE:HD13	2:A:437:TYR:HB3	1.48	0.96
2:A:403:LEU:HD13	2:A:409:VAL:HG22	1.54	0.90
2:A:106:LEU:HD21	2:A:214:THR:HG23	1.56	0.88
1:B:921:A:N6	1:B:946:G:H2'	1.92	0.84
1:B:939:U:H2'	1:B:940:C:C6	2.11	0.83
1:B:939:U:C2	1:B:940:C:C6	2.69	0.81
1:B:920:U:H2'	1:B:920:U:O2	1.81	0.79
1:B:933:U:H2'	1:B:935:U:OP1	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:471:LEU:HB2	2:A:497:VAL:HG13	1.66	0.78
2:A:391:ASP:HA	2:A:402:ARG:HD2	1.65	0.77
2:A:39:LEU:HD13	2:A:81:ILE:HG12	1.68	0.76
2:A:341:ARG:HD3	2:A:369:PRO:HD2	1.69	0.75
1:B:919:G:C1'	1:B:920:U:C5	2.71	0.71
2:A:362:MET:CG	2:A:378:GLN:HG3	2.14	0.71
2:A:394:GLU:HA	2:A:405:LEU:HB2	1.73	0.70
2:A:32:PRO:HA	2:A:64:ARG:O	1.90	0.70
2:A:424:LYS:HD3	2:A:428:GLY:O	1.92	0.70
1:B:921:A:C6	1:B:948:U:C6	2.79	0.70
2:A:457:HIS:HD2	2:A:520:ARG:HE	1.39	0.70
1:B:903:G:O2'	1:B:904:G:H5'	1.92	0.69
2:A:352:VAL:HG12	2:A:384:GLU:HG2	1.73	0.69
2:A:362:MET:HG2	2:A:378:GLN:CG	2.15	0.68
2:A:229:CYS:O	2:A:257:GLU:HA	1.94	0.68
1:B:958:A:O2'	1:B:960:U:C5	2.47	0.68
1:B:935:U:C5	1:B:937:A:C2	2.82	0.67
2:A:159:LYS:HD3	2:A:164:GLY:HA3	1.77	0.67
1:B:976:A:C2	2:A:233:PHE:CZ	2.83	0.66
1:B:918:G:C4'	1:B:919:G:OP1	2.40	0.66
2:A:43:HIS:O	2:A:47:ILE:HG13	1.95	0.66
1:B:919:G:H4'	1:B:920:U:H6	1.61	0.66
2:A:26:THR:HB	5:A:1451:HOH:O	1.97	0.65
2:A:355:ASN:HB2	2:A:436:THR:HG22	1.78	0.65
1:B:921:A:C5	1:B:948:U:C5	2.85	0.65
1:B:935:U:O2	2:A:519:GLU:HG3	1.97	0.64
1:B:939:U:C2	1:B:940:C:C5	2.85	0.64
2:A:463:HIS:O	2:A:505:PRO:HD3	1.98	0.64
2:A:410:ARG:HD3	2:A:416:VAL:HG22	1.79	0.64
2:A:75:ILE:O	2:A:79:GLU:HG3	1.98	0.64
1:B:919:G:C4	1:B:957:G:N2	2.66	0.63
2:A:159:LYS:HD2	2:A:165:PHE:CD2	2.33	0.63
2:A:82:LYS:HD3	2:A:96:VAL:HG21	1.79	0.63
2:A:173:ARG:HD2	2:A:187:ASP:O	1.97	0.63
2:A:192:ARG:HD3	2:A:194:LYS:HE3	1.79	0.63
2:A:433:ILE:HG22	2:A:435:CYS:SG	2.38	0.63
1:B:937:A:C2	1:B:938:U:H1'	2.32	0.63
2:A:28:HIS:HE1	2:A:62:ASN:OD1	1.81	0.62
2:A:522:GLY:HA2	2:A:544:LEU:HD12	1.81	0.62
2:A:391:ASP:O	2:A:402:ARG:HB3	2.00	0.62
2:A:149:SER:OG	2:A:152:GLU:HG3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:918:G:O2'	1:B:957:G:N2	2.32	0.62
2:A:346:ILE:HD13	2:A:521:GLU:OE1	2.00	0.62
1:B:916:C:H3'	1:B:916:C:O2	1.99	0.62
2:A:380:PRO:HB2	2:A:463:HIS:CE1	2.35	0.61
1:B:958:A:O2'	1:B:960:U:H5	1.84	0.61
1:B:963:U:H2'	1:B:964:C:C6	2.36	0.61
2:A:412:ARG:HB2	2:A:457:HIS:HA	1.82	0.61
1:B:902:G:C8	2:A:137:THR:HG22	2.36	0.61
2:A:121:VAL:HG21	2:A:156:LEU:HB3	1.83	0.61
1:B:937:A:H2'	1:B:938:U:O4'	2.00	0.61
2:A:298:ARG:HE	2:A:528:SER:HA	1.66	0.60
2:A:467:VAL:HG21	2:A:503:ALA:HB3	1.83	0.60
2:A:270:LYS:O	2:A:274:ASN:HB2	2.02	0.60
2:A:403:LEU:HD13	2:A:409:VAL:CG2	2.30	0.59
1:B:976:A:C2	2:A:233:PHE:CE1	2.90	0.59
2:A:167:GLU:HG3	2:A:195:PHE:HD2	1.67	0.59
1:B:909:C:O2'	1:B:945:G:H2'	2.02	0.59
1:B:957:G:H2'	1:B:958:A:H5'	1.85	0.59
2:A:419:ALA:O	2:A:420:GLU:HG3	2.02	0.59
2:A:397:ASN:ND2	2:A:400:TYR:HB2	2.19	0.58
2:A:40:HIS:CE1	2:A:268:MET:HG3	2.38	0.58
2:A:401:LYS:O	2:A:454:GLY:HA3	2.03	0.58
1:B:920:U:C2'	1:B:920:U:O2	2.50	0.57
1:B:916:C:H1'	1:B:960:U:O2'	2.04	0.57
2:A:393:ARG:HB2	2:A:400:TYR:CZ	2.39	0.57
2:A:393:ARG:O	2:A:404:VAL:HA	2.03	0.57
2:A:351:LEU:HD23	2:A:352:VAL:N	2.19	0.57
2:A:132:TYR:CD2	2:A:141:LYS:HG3	2.39	0.57
2:A:230:THR:HG21	2:A:260:ARG:HB3	1.87	0.56
2:A:526:LEU:HG	2:A:527:ASP:H	1.68	0.56
2:A:534:GLU:O	2:A:536:PRO:HD3	2.05	0.56
2:A:507:LEU:HD12	2:A:538:PHE:CE2	2.40	0.56
2:A:392:PHE:HZ	2:A:405:LEU:HD13	1.68	0.56
2:A:166:GLU:O	2:A:169:LYS:HB2	2.06	0.56
1:B:956:C:O5'	1:B:956:C:H6	1.88	0.55
2:A:144:PRO:HG2	2:A:145:TYR:CE2	2.41	0.55
1:B:910:G:N7	1:B:945:G:N2	2.55	0.55
2:A:265:TYR:CZ	2:A:479:PRO:HG3	2.41	0.55
1:B:930:G:O2'	1:B:931:A:H5'	2.06	0.55
2:A:468:GLU:HB2	2:A:535:LYS:HE3	1.88	0.55
2:A:35:PRO:O	2:A:77:TYR:HD2	1.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:410:ARG:HD3	2:A:416:VAL:CG2	2.37	0.54
2:A:64:ARG:HD3	2:A:222:GLU:OE2	2.08	0.54
2:A:465:LEU:HD21	2:A:536:PRO:HG2	1.88	0.54
2:A:343:MET:HE1	2:A:412:ARG:CB	2.38	0.54
2:A:136:LEU:HD23	2:A:183:ILE:CD1	2.37	0.54
2:A:30:ARG:NH1	2:A:215:HIS:NE2	2.56	0.54
2:A:41:ILE:HD11	2:A:309:PHE:CD2	2.43	0.54
1:B:934:C:O2'	2:A:412:ARG:NH1	2.40	0.53
1:B:922:A:H3'	1:B:923:G:H8	1.73	0.53
2:A:231:LEU:O	2:A:234:GLN:HG3	2.08	0.53
2:A:282:VAL:HG12	2:A:289:ARG:HH11	1.73	0.53
2:A:487:PHE:O	2:A:490:VAL:HG12	2.08	0.53
2:A:65:PHE:HE2	2:A:96:VAL:HG11	1.74	0.53
1:B:943:G:H2'	1:B:944:A:C8	2.43	0.53
2:A:106:LEU:CD2	2:A:214:THR:HG23	2.36	0.53
2:A:28:HIS:CE1	2:A:62:ASN:OD1	2.60	0.53
2:A:408:GLU:O	2:A:409:VAL:HG13	2.09	0.52
2:A:351:LEU:HD11	2:A:417:ILE:HD12	1.92	0.52
1:B:954:U:H6	1:B:954:U:O5'	1.91	0.52
2:A:422:VAL:HG22	2:A:423:GLU:H	1.75	0.52
2:A:424:LYS:HA	2:A:430:ILE:HA	1.92	0.52
2:A:529:ARG:HG3	2:A:529:ARG:O	2.10	0.52
1:B:916:C:C2'	1:B:918:G:OP2	2.58	0.51
1:B:918:G:N2	1:B:955:U:O2	2.38	0.51
2:A:348:PRO:HA	2:A:387:ILE:O	2.11	0.51
1:B:951:A:H2'	1:B:952:G:O5'	2.10	0.51
1:B:959:A:C5	1:B:960:U:C4	2.98	0.51
2:A:351:LEU:HD11	2:A:417:ILE:CD1	2.40	0.51
1:B:937:A:C4	1:B:938:U:C6	2.99	0.51
2:A:59:GLY:HA2	5:A:1451:HOH:O	2.10	0.51
2:A:299:ARG:O	2:A:299:ARG:HG3	2.09	0.51
1:B:955:U:H2'	1:B:957:G:OP2	2.09	0.51
1:B:963:U:O2'	1:B:964:C:H5'	2.10	0.51
2:A:357:GLN:NE2	5:A:1454:HOH:O	2.44	0.51
2:A:425:ASP:OD1	2:A:429:ASN:HB2	2.11	0.51
2:A:347:ASP:O	2:A:388:ASP:HA	2.10	0.51
2:A:500:GLN:HA	2:A:500:GLN:OE1	2.09	0.51
2:A:531:SER:HB3	2:A:537:VAL:H	1.76	0.50
1:B:937:A:C5	1:B:938:U:C6	2.99	0.50
1:B:956:C:H2'	1:B:957:G:O4'	2.11	0.50
1:B:919:G:C4'	1:B:920:U:H6	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:392:PHE:CZ	2:A:405:LEU:HD13	2.45	0.50
2:A:356:TYR:HA	2:A:437:TYR:CE1	2.46	0.50
2:A:460:SER:O	2:A:464:ALA:HB2	2.12	0.50
2:A:381:PHE:CD1	2:A:382:SER:N	2.80	0.50
2:A:46:SER:HB2	4:A:998:A:H1'	1.94	0.50
2:A:115:ASN:HD21	2:A:154:LEU:HD21	1.75	0.49
1:B:974:C:H1'	2:A:192:ARG:HB3	1.94	0.49
2:A:260:ARG:HB2	4:A:998:A:C6	2.47	0.49
2:A:227:SER:O	2:A:255:GLN:HA	2.12	0.49
2:A:262:ASN:HB2	2:A:320:ASN:O	2.12	0.49
2:A:272:LYS:HD2	3:A:1395:SO4:O1	2.12	0.49
1:B:910:G:C6	1:B:926:A:C2	3.00	0.49
2:A:505:PRO:HG2	5:A:1474:HOH:O	2.11	0.49
2:A:419:ALA:HA	2:A:435:CYS:SG	2.53	0.49
2:A:136:LEU:HD23	2:A:183:ILE:HD11	1.95	0.49
1:B:929:G:C2	1:B:942:G:C4	3.01	0.48
2:A:263:LEU:HB3	2:A:266:THR:CG2	2.43	0.48
2:A:488:LEU:O	2:A:491:ILE:HG13	2.13	0.48
2:A:365:MET:SD	2:A:413:ASN:HB2	2.53	0.48
2:A:407:LYS:HE3	2:A:408:GLU:HG3	1.95	0.48
2:A:531:SER:HB3	2:A:537:VAL:N	2.29	0.48
2:A:424:LYS:HG2	2:A:430:ILE:HG12	1.96	0.48
2:A:412:ARG:HH11	2:A:412:ARG:HG2	1.79	0.48
2:A:265:TYR:CD1	2:A:474:ARG:HD3	2.49	0.48
1:B:918:G:H1	1:B:955:U:H1'	1.79	0.47
2:A:412:ARG:NH1	2:A:412:ARG:HG2	2.29	0.47
2:A:167:GLU:HG3	2:A:195:PHE:CD2	2.47	0.47
2:A:301:TYR:CE2	2:A:331:ILE:HB	2.50	0.47
2:A:307:ARG:NH2	3:A:1396:SO4:S	2.88	0.47
2:A:81:ILE:O	2:A:85:VAL:HG23	2.13	0.47
1:B:904:G:C2	1:B:970:C:C2	3.02	0.47
2:A:37:GLY:N	2:A:77:TYR:CD2	2.83	0.47
1:B:957:G:C2'	1:B:958:A:H5'	2.44	0.47
2:A:422:VAL:HG13	2:A:423:GLU:N	2.30	0.47
2:A:464:ALA:O	2:A:466:PRO:HD3	2.15	0.47
2:A:343:MET:HB3	2:A:343:MET:HE3	1.71	0.47
2:A:40:HIS:HA	2:A:292:THR:HA	1.96	0.47
1:B:919:G:C1'	1:B:920:U:H5	2.07	0.46
2:A:159:LYS:HD2	2:A:165:PHE:CE2	2.49	0.46
1:B:955:U:C2'	1:B:957:G:N7	2.79	0.46
2:A:267:VAL:HB	3:A:1395:SO4:O1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:935:U:C2	2:A:519:GLU:HG3	2.49	0.46
2:A:260:ARG:HB2	4:A:998:A:N1	2.30	0.46
2:A:123:GLU:HG3	2:A:148:ARG:NH2	2.30	0.46
1:B:948:U:C2	1:B:959:A:O4'	2.69	0.46
1:B:968:C:O2'	1:B:969:C:H5'	2.16	0.46
2:A:41:ILE:HG21	2:A:263:LEU:HD12	1.97	0.46
1:B:908:U:C4	1:B:913:A:C5	3.03	0.46
1:B:955:U:O2'	1:B:957:G:N7	2.46	0.46
1:B:919:G:C5	1:B:957:G:N2	2.84	0.46
1:B:952:G:N2	1:B:963:U:C2	2.83	0.46
2:A:415:TYR:CE1	2:A:442:LEU:HD22	2.51	0.46
1:B:955:U:C6	1:B:957:G:OP2	2.68	0.45
2:A:346:ILE:HG23	2:A:499:LYS:CB	2.46	0.45
1:B:916:C:O2	1:B:916:C:C2'	2.64	0.45
1:B:916:C:H4'	1:B:960:U:O2	2.15	0.45
1:B:941:C:C2	1:B:942:G:C8	3.05	0.45
2:A:478:VAL:O	2:A:481:PRO:HD3	2.15	0.45
1:B:957:G:H8	1:B:957:G:O5'	2.00	0.45
1:B:939:U:N3	1:B:940:C:C5	2.84	0.45
2:A:390:ALA:O	2:A:402:ARG:NH1	2.50	0.45
1:B:934:C:N4	2:A:410:ARG:HE	2.15	0.45
1:B:973:G:OP2	2:A:130:ARG:HG3	2.17	0.45
1:B:969:C:O2'	1:B:970:C:H5'	2.17	0.45
2:A:273:LEU:O	2:A:277:VAL:HG23	2.17	0.45
2:A:33:PRO:HG3	2:A:81:ILE:HG21	1.99	0.45
2:A:336:ASN:O	2:A:368:HIS:HE1	2.00	0.45
1:B:961:C:O2'	1:B:962:C:H5'	2.16	0.45
2:A:478:VAL:HA	2:A:479:PRO:HD3	1.87	0.44
2:A:30:ARG:NH2	2:A:228:LEU:O	2.50	0.44
2:A:106:LEU:HD12	2:A:217:ILE:HG21	1.99	0.44
1:B:951:A:C2'	1:B:952:G:O5'	2.66	0.44
2:A:518:PHE:HZ	2:A:538:PHE:CD2	2.36	0.44
2:A:522:GLY:H	2:A:524:PHE:HE1	1.66	0.44
2:A:528:SER:O	2:A:530:HIS:CD2	2.70	0.44
2:A:47:ILE:HG23	2:A:51:PHE:CD2	2.51	0.44
1:B:934:C:H41	2:A:410:ARG:HH21	1.64	0.44
2:A:144:PRO:HG2	2:A:145:TYR:CD2	2.52	0.44
1:B:958:A:O2'	1:B:960:U:C6	2.66	0.44
1:B:933:U:H2'	1:B:935:U:P	2.58	0.43
2:A:407:LYS:HG3	2:A:408:GLU:H	1.83	0.43
1:B:904:G:N2	1:B:970:C:C2	2.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:65:PHE:CE1	2:A:78:VAL:HA	2.53	0.43
2:A:180:SER:O	2:A:186:ARG:NH1	2.51	0.43
2:A:35:PRO:HG2	2:A:73:GLU:HB3	2.00	0.43
2:A:273:LEU:HA	2:A:276:LEU:HD12	2.01	0.43
2:A:392:PHE:HE2	2:A:430:ILE:CD1	2.31	0.43
1:B:939:U:O2	1:B:940:C:C6	2.70	0.43
1:B:943:G:O2'	1:B:944:A:O5'	2.27	0.43
2:A:491:ILE:HG22	2:A:492:ASN:N	2.34	0.43
2:A:176:ILE:HG22	2:A:177:ASP:N	2.34	0.43
1:B:916:C:C3'	1:B:916:C:O2	2.64	0.43
2:A:524:PHE:N	2:A:524:PHE:CD1	2.87	0.43
2:A:77:TYR:O	2:A:81:ILE:HG13	2.19	0.43
2:A:377:ARG:HH11	2:A:377:ARG:HG2	1.84	0.43
2:A:230:THR:HA	2:A:258:PHE:O	2.18	0.43
2:A:231:LEU:HD21	2:A:317:LYS:O	2.18	0.43
2:A:385:ILE:HA	2:A:460:SER:HA	2.00	0.43
2:A:346:ILE:HG13	2:A:469:ILE:CD1	2.49	0.42
1:B:954:U:C4	1:B:955:U:C4	3.07	0.42
2:A:474:ARG:HE	2:A:474:ARG:HB3	1.72	0.42
2:A:353:ILE:HG21	2:A:437:TYR:CD1	2.54	0.42
1:B:954:U:C6	1:B:954:U:O5'	2.72	0.42
2:A:346:ILE:HG13	2:A:469:ILE:HD12	2.01	0.42
2:A:301:TYR:CE2	2:A:327:LEU:HD22	2.55	0.42
1:B:939:U:C2'	1:B:940:C:H6	2.12	0.42
2:A:263:LEU:HD22	2:A:324:MET:HE2	2.01	0.42
1:B:932:U:C4	1:B:933:U:C4	3.07	0.42
2:A:507:LEU:HD12	2:A:538:PHE:CZ	2.54	0.42
1:B:929:G:C6	1:B:942:G:C6	3.08	0.42
2:A:364:THR:HA	2:A:377:ARG:O	2.20	0.42
1:B:937:A:O2'	2:A:544:LEU:HD23	2.19	0.42
2:A:282:VAL:HG12	2:A:289:ARG:NH1	2.34	0.42
2:A:340:PRO:HA	2:A:367:ASN:O	2.20	0.42
1:B:953:G:C2	1:B:962:C:C2	3.07	0.41
2:A:354:GLU:OE1	2:A:434:PHE:HB3	2.20	0.41
2:A:361:GLU:HG3	2:A:362:MET:N	2.35	0.41
2:A:434:PHE:N	2:A:434:PHE:CD1	2.87	0.41
1:B:910:G:C5	1:B:926:A:C2	3.08	0.41
2:A:365:MET:SD	2:A:413:ASN:OD1	2.78	0.41
2:A:129:ILE:O	2:A:133:ARG:HB2	2.19	0.41
2:A:430:ILE:HG22	2:A:431:THR:N	2.34	0.41
2:A:114:ILE:CG2	2:A:154:LEU:HD13	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:472:TYR:CE1	2:A:496:LEU:HD13	2.55	0.41
2:A:343:MET:SD	2:A:412:ARG:HG3	2.60	0.41
2:A:270:LYS:HZ1	4:A:998:A:P	2.42	0.41
2:A:507:LEU:HD12	2:A:538:PHE:HE2	1.81	0.41
1:B:924:G:O2'	2:A:312:ARG:HD3	2.20	0.41
2:A:407:LYS:HG3	2:A:408:GLU:N	2.34	0.41
2:A:528:SER:O	2:A:529:ARG:HB3	2.21	0.41
2:A:114:ILE:HD11	2:A:172:LEU:HD11	2.02	0.41
2:A:392:PHE:HA	2:A:403:LEU:HB3	2.03	0.41
2:A:341:ARG:HD2	2:A:368:HIS:HA	2.01	0.41
1:B:955:U:H2'	1:B:957:G:N7	2.35	0.41
2:A:422:VAL:HG21	2:A:430:ILE:HD13	2.02	0.41
2:A:528:SER:HB3	2:A:539:ASN:OD1	2.20	0.41
2:A:464:ALA:HB1	2:A:502:PHE:HB3	2.03	0.41
2:A:11:ILE:O	2:A:15:ILE:HG13	2.21	0.41
1:B:921:A:C4	1:B:948:U:C5	3.09	0.41
2:A:522:GLY:N	2:A:524:PHE:HE1	2.19	0.41
1:B:938:U:O2	1:B:938:U:H2'	2.21	0.41
2:A:46:SER:CB	4:A:998:A:H1'	2.50	0.41
2:A:343:MET:HE1	2:A:412:ARG:HB2	2.03	0.40
2:A:230:THR:CG2	2:A:260:ARG:HB3	2.51	0.40
1:B:916:C:H2'	1:B:918:G:OP2	2.21	0.40
2:A:389:ARG:O	2:A:391:ASP:N	2.53	0.40
2:A:69:ASN:HA	2:A:70:PRO:HD2	1.84	0.40
1:B:955:U:N1	1:B:957:G:OP2	2.55	0.40
1:B:919:G:C1'	1:B:920:U:C6	3.05	0.40
2:A:518:PHE:CD1	2:A:518:PHE:N	2.89	0.40
2:A:19:LEU:HA	2:A:19:LEU:HD12	1.78	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	525/548 (96%)	463 (88%)	51 (10%)	11 (2%)	9	23

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	32	PRO
2	A	397	ASN
2	A	422	VAL
2	A	531	SER
2	A	390	ALA
2	A	526	LEU
2	A	283	GLU
2	A	413	ASN
2	A	400	TYR
2	A	405	LEU
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	463/478 (97%)	420 (91%)	43 (9%)	11	25

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

Mol	Chain	Res	Type
2	A	19	LEU
2	A	27	VAL
2	A	30	ARG
2	A	32	PRO
2	A	49	LEU
2	A	66	ASP
2	A	73	GLU
2	A	78	VAL
2	A	80	SER
2	A	100	SER

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Mol	Chain	Res	Type
2	A	105	GLN
2	A	106	LEU
2	A	124	LEU
2	A	154	LEU
2	A	156	LEU
2	A	159	LYS
2	A	186	ARG
2	A	192	ARG
2	A	206	CYS
2	A	231	LEU
2	A	232	GLU
2	A	249	ILE
2	A	327	LEU
2	A	335	LEU
2	A	336	ASN
2	A	341	ARG
2	A	362	MET
2	A	365	MET
2	A	369	PRO
2	A	395	GLU
2	A	397	ASN
2	A	398	LYS
2	A	408	GLU
2	A	409	VAL
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	516	PHE
2	A	519	GLU
2	A	528	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	28	HIS
2	A	115	ASN
2	A	153	ASN
2	A	226	HIS
2	A	236	ASN

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Mol	Chain	Res	Type
2	A	355	ASN
2	A	368	HIS
2	A	397	ASN
2	A	413	ASN
2	A	457	HIS
2	A	530	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	72/73 (98%)	19 (26%)	12 (16%)

All (19) 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	918	G
1	B	919	G
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	944	A
1	B	945	G
1	B	949	C
1	B	959	A
1	B	961	C
1	B	973	G
1	B	974	C

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	907	A
1	B	909	C
1	B	916	C

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Mol	Chain	Res	Type
1	B	918	G
1	B	934	C
1	B	935	U
1	B	936	G
1	B	943	G
1	B	948	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 carbohydrates 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	1.62	1 (25%)	6,6,6	0.50	0
3	SO4	A	1396	-	4,4,4	1.69	1 (25%)	6,6,6	0.53	0
4	A	A	998	-	15,24,25	0.67	0	16,35,38	0.58	0
3	SO4	B	1393	-	4,4,4	1.63	1 (25%)	6,6,6	0.51	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
3	SO4	A	1395	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1396	-	-	0/0/0/0	0/0/0/0
4	A	A	998	-	-	0/3/25/26	0/3/3/3
3	SO4	B	1393	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1395	SO4	O3-S	2.11	1.55	1.47
3	B	1393	SO4	O3-S	2.37	1.55	1.47
3	A	1396	SO4	O3-S	2.44	1.56	1.47

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 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1395	SO4	2	0
3	A	1396	SO4	1	0
4	A	998	A	5	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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.