



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 06:59 PM EDT

PDB ID : 2DR2  
Title : Structure of human tryptophanyl-tRNA synthetase in complex with tRNA(Trp)  
Authors : Shen, N.; Guo, L.; Yang, B.; Jin, Y.; Ding, J.  
Deposited on : 2006-06-05  
Resolution : 3.00 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

<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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

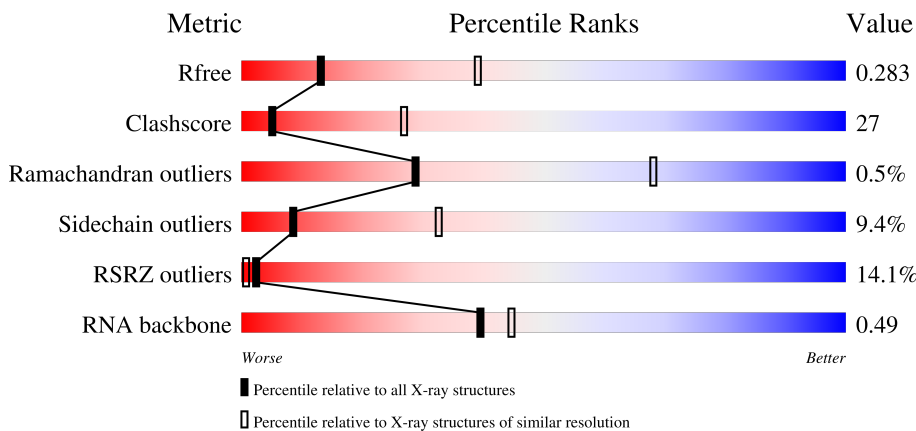
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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  $\geq 3$ , 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	81% 24% 56% 19% •
2	A	384	% 53% 38% 6% •

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4638 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 transfer RNA-Trp.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	B	75	1603	714	287	527	75	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	373	3015	1934	510	556	15	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

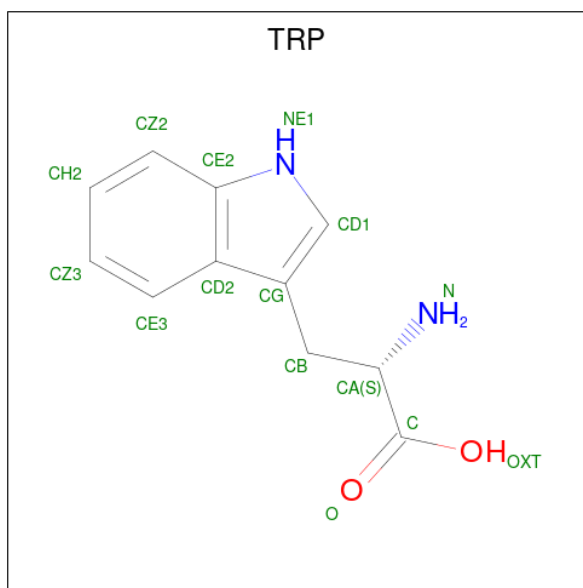
Chain	Residue	Modelled	Actual	Comment	Reference
A	472	HIS	-	expression tag	UNP P23381
A	473	HIS	-	expression tag	UNP P23381
A	474	HIS	-	expression tag	UNP P23381
A	475	HIS	-	expression tag	UNP P23381
A	476	HIS	-	expression tag	UNP P23381
A	477	HIS	-	expression tag	UNP P23381

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is TRYPTOPHAN (three-letter code: TRP) (formula:  $C_{11}H_{12}N_2O_2$ ).

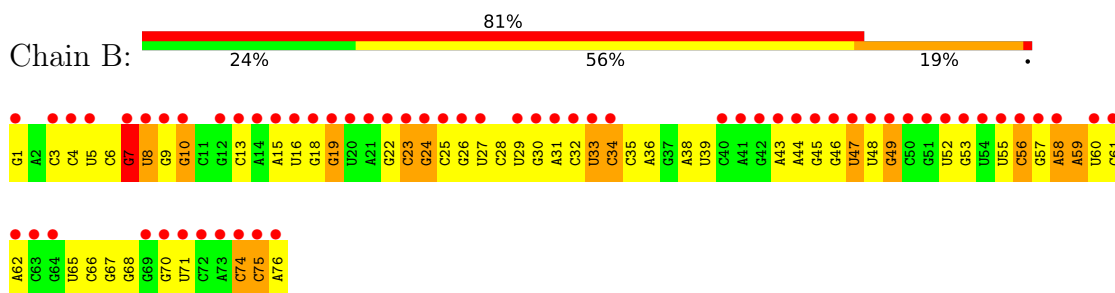


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
4	A	1	Total	C	N	O	0	0
			15	11	2	2		

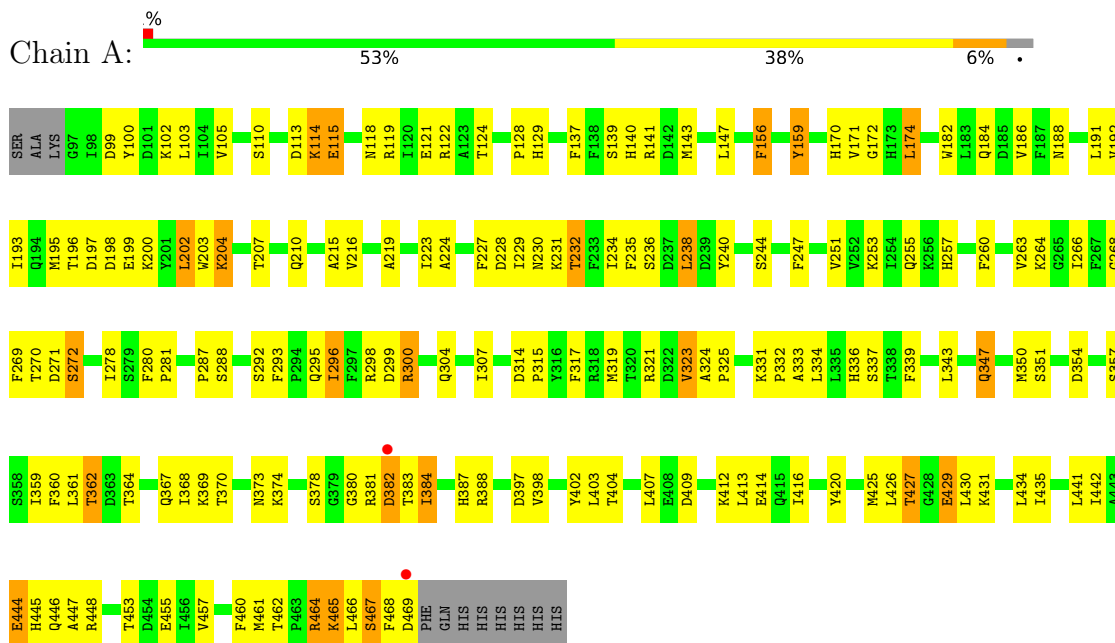
### 3 Residue-property plots i

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 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.

- Molecule 1: transfer RNA-Trp



- Molecule 2: Tryptophanyl-tRNA synthetase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.30Å 132.30Å 137.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.10 – 3.00 44.10 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.10-3.00) 99.8 (44.10-3.00)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.64 (at 3.01Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.228 , 0.285 0.227 , 0.283	Depositor DCC
$R_{free}$ test set	1254 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.7	Xtrriage
Anisotropy	0.240	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 65.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.008 for -h,l,k 0.007 for -l,-k,-h	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	4638	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.32	1/1791 (0.1%)	0.68	1/2789 (0.0%)
2	A	0.45	0/3088	0.66	0/4166
All	All	0.41	1/4879 (0.0%)	0.67	1/6955 (0.0%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	G	OP3-P	-7.58	1.52	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	7	G	N9-C1'-C2'	5.31	120.90	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	7	G	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	1603	0	810	73	0
2	A	3015	0	2974	166	0
3	A	5	0	0	0	0
4	A	15	0	9	0	0
All	All	4638	0	3793	228	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 (228) 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:465:LYS:H	2:A:465:LYS:HD3	1.05	1.10
2:A:207:THR:HG22	2:A:210:GLN:HG3	1.41	1.02
1:B:32:C:H2'	1:B:33:U:H5''	1.43	1.01
2:A:118:ASN:HB3	2:A:122:ARG:HH21	1.35	0.92
2:A:465:LYS:H	2:A:465:LYS:CD	1.82	0.90
1:B:55:U:H2'	1:B:56:C:H5''	1.54	0.88
2:A:465:LYS:HD3	2:A:465:LYS:N	1.89	0.87
2:A:380:GLY:HA3	2:A:427:THR:HG21	1.55	0.87
1:B:58:A:H1'	1:B:60:U:H5	1.38	0.85
1:B:32:C:C2'	1:B:33:U:H5''	2.06	0.85
2:A:198:ASP:HB3	2:A:238:LEU:HD13	1.57	0.83
2:A:296:ILE:HD12	2:A:466:LEU:HD12	1.63	0.80
2:A:159:TYR:CZ	2:A:287:PRO:HG2	2.18	0.78
2:A:460:PHE:HA	2:A:464:ARG:NH2	1.99	0.77
2:A:99:ASP:OD2	2:A:102:LYS:HB3	1.84	0.77
1:B:34:C:H42	2:A:427:THR:HG23	1.49	0.76
2:A:207:THR:HG22	2:A:210:GLN:CG	2.15	0.75
2:A:380:GLY:HA3	2:A:427:THR:CG2	2.16	0.75
2:A:293:PHE:HB3	2:A:296:ILE:HG23	1.69	0.74
2:A:207:THR:CG2	2:A:210:GLN:HG3	2.17	0.74
2:A:174:LEU:HD22	2:A:361:LEU:HD21	1.70	0.74
2:A:416:ILE:HA	2:A:425:MET:HE1	1.69	0.73
2:A:260:PHE:CE2	2:A:278:ILE:HD12	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:364:THR:O	2:A:368:ILE:HG12	1.89	0.73
2:A:369:LYS:HA	2:A:435:ILE:HD13	1.72	0.72
2:A:216:VAL:HG22	2:A:461:MET:HE1	1.69	0.72
2:A:347:GLN:CD	2:A:347:GLN:H	1.91	0.72
2:A:442:ILE:O	2:A:446:GLN:HG3	1.90	0.71
2:A:139:SER:HB3	2:A:336:HIS:HB2	1.71	0.71
2:A:228:ASP:O	2:A:232:THR:HG23	1.89	0.71
2:A:113:ASP:OD1	2:A:115:GLU:HG2	1.91	0.71
1:B:60:U:H5''	1:B:61:C:OP2	1.91	0.70
2:A:253:LYS:O	2:A:257:HIS:HD2	1.74	0.70
1:B:58:A:H1'	1:B:60:U:C5	2.25	0.69
2:A:460:PHE:HA	2:A:464:ARG:HH22	1.55	0.69
1:B:22:G:H2'	1:B:23:C:H1'	1.77	0.66
1:B:55:U:C2'	1:B:56:C:H5''	2.24	0.66
2:A:140:HIS:HD2	2:A:143:MET:H	1.44	0.66
1:B:25:C:O2'	1:B:26:G:H5'	1.96	0.65
2:A:464:ARG:HH11	2:A:466:LEU:HD21	1.60	0.65
2:A:464:ARG:NH1	2:A:466:LEU:HD21	2.11	0.65
1:B:33:U:H2'	1:B:34:C:H5''	1.78	0.64
1:B:34:C:P	2:A:384:ILE:HG22	2.38	0.64
2:A:115:GLU:CD	2:A:115:GLU:H	1.99	0.64
2:A:184:GLN:OE1	2:A:232:THR:HG22	1.98	0.63
2:A:118:ASN:HB3	2:A:122:ARG:NH2	2.11	0.63
2:A:227:PHE:HB3	2:A:232:THR:HG21	1.79	0.63
2:A:170:HIS:HD2	2:A:172:GLY:H	1.47	0.62
1:B:4:C:H2'	1:B:5:U:H6	1.64	0.62
1:B:22:G:H2'	1:B:23:C:C1'	2.30	0.62
2:A:188:ASN:ND2	2:A:231:LYS:HE2	2.16	0.61
1:B:33:U:H5'	1:B:33:U:H6	1.65	0.61
2:A:251:VAL:O	2:A:255:GLN:HG3	2.01	0.61
2:A:198:ASP:O	2:A:202:LEU:HD22	2.00	0.61
2:A:321:ARG:O	2:A:331:LYS:HE2	2.01	0.61
2:A:370:THR:HG23	2:A:374:LYS:HD2	1.83	0.60
2:A:298:ARG:O	2:A:298:ARG:HG2	2.01	0.60
2:A:170:HIS:HA	2:A:360:PHE:HA	1.84	0.59
2:A:191:LEU:HD12	2:A:192:VAL:H	1.67	0.59
2:A:192:VAL:HG13	2:A:235:PHE:HE1	1.66	0.59
1:B:57:G:O2'	1:B:58:A:H5'	2.02	0.59
2:A:425:MET:HG3	2:A:429:GLU:HG3	1.85	0.59
1:B:19:G:OP2	1:B:19:G:H8	1.86	0.58
2:A:324:ALA:HB3	2:A:325:PRO:HD3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:140:HIS:CD2	2:A:143:MET:H	2.20	0.58
2:A:260:PHE:HE2	2:A:278:ILE:HD12	1.69	0.58
2:A:453:THR:OG1	2:A:455:GLU:HG2	2.04	0.57
2:A:426:LEU:O	2:A:429:GLU:HG3	2.03	0.57
2:A:464:ARG:HH11	2:A:466:LEU:CD2	2.17	0.57
1:B:28:C:H2'	1:B:29:U:C6	2.40	0.56
1:B:34:C:OP1	2:A:383:THR:HA	2.04	0.56
2:A:234:ILE:O	2:A:461:MET:HA	2.06	0.56
2:A:359:ILE:N	2:A:359:ILE:HD12	2.21	0.56
1:B:34:C:H42	2:A:427:THR:CG2	2.18	0.56
1:B:23:C:C4	1:B:25:C:N4	2.74	0.56
1:B:3:C:H2'	1:B:4:C:C6	2.41	0.56
2:A:293:PHE:HB3	2:A:296:ILE:CG2	2.36	0.56
1:B:44:A:O2'	1:B:45:G:H5'	2.06	0.55
1:B:49:G:H5'	1:B:49:G:H8	1.72	0.55
1:B:34:C:N4	2:A:427:THR:HG23	2.20	0.54
1:B:9:G:H4'	1:B:47:U:OP2	2.07	0.54
1:B:30:G:O2'	1:B:31:A:H5'	2.07	0.54
2:A:137:PHE:CZ	2:A:337:SER:HB3	2.43	0.54
2:A:317:PHE:O	2:A:321:ARG:HG3	2.08	0.54
1:B:34:C:OP2	2:A:384:ILE:HG22	2.08	0.54
2:A:102:LYS:HZ3	2:A:105:VAL:HG11	1.72	0.54
2:A:445:HIS:HD2	2:A:448:ARG:HH21	1.56	0.54
2:A:199:GLU:HB2	2:A:280:PHE:CZ	2.42	0.54
2:A:300:ARG:NH1	2:A:300:ARG:HG2	2.23	0.54
2:A:247:PHE:HD1	2:A:292:SER:HB3	1.73	0.53
2:A:460:PHE:CA	2:A:464:ARG:NH2	2.71	0.53
1:B:10:G:H3'	1:B:10:G:OP2	2.08	0.53
2:A:409:ASP:CG	2:A:412:LYS:HG3	2.29	0.53
2:A:403:LEU:HD21	2:A:434:LEU:HA	1.91	0.53
1:B:25:C:H2'	1:B:26:G:O4'	2.09	0.53
2:A:362:THR:HA	2:A:446:GLN:HE21	1.74	0.53
1:B:61:C:H2'	1:B:62:A:H8	1.74	0.52
2:A:431:LYS:O	2:A:435:ILE:HG13	2.09	0.52
2:A:427:THR:O	2:A:431:LYS:HG3	2.10	0.52
1:B:67:G:H2'	1:B:68:G:H8	1.74	0.52
2:A:350:MET:HA	2:A:357:SER:OG	2.10	0.52
1:B:8:U:O2	1:B:8:U:H2'	2.10	0.51
1:B:3:C:H2'	1:B:4:C:H6	1.74	0.51
2:A:110:SER:HB2	2:A:140:HIS:CE1	2.46	0.51
1:B:4:C:H2'	1:B:5:U:C6	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:C:O2'	1:B:24:G:H5''	2.11	0.51
2:A:195:MET:HB2	2:A:236:SER:HA	1.91	0.51
2:A:314:ASP:N	2:A:315:PRO:HD2	2.25	0.51
2:A:102:LYS:NZ	2:A:105:VAL:HG11	2.24	0.50
2:A:156:PHE:HA	2:A:304:GLN:O	2.11	0.50
2:A:370:THR:CG2	2:A:374:LYS:HD2	2.41	0.50
2:A:462:THR:O	2:A:464:ARG:HG3	2.12	0.50
2:A:263:VAL:HB	2:A:269:PHE:CE2	2.46	0.50
2:A:198:ASP:HB3	2:A:238:LEU:CD1	2.34	0.50
2:A:191:LEU:HD12	2:A:192:VAL:N	2.26	0.50
2:A:347:GLN:OE1	2:A:347:GLN:N	2.45	0.50
2:A:359:ILE:HD13	2:A:402:TYR:CE2	2.47	0.50
2:A:414:GLU:OE1	2:A:414:GLU:HA	2.12	0.49
2:A:118:ASN:CB	2:A:122:ARG:HH21	2.17	0.49
2:A:193:ILE:HD12	2:A:234:ILE:HD13	1.94	0.49
2:A:445:HIS:HD2	2:A:448:ARG:NH2	2.10	0.49
1:B:32:C:C3'	1:B:33:U:H5''	2.42	0.49
2:A:204:LYS:HA	2:A:204:LYS:HZ2	1.77	0.49
2:A:378:SER:HA	2:A:397:ASP:OD1	2.12	0.49
1:B:36:A:H5'	2:A:373:ASN:O	2.11	0.49
2:A:102:LYS:HA	2:A:105:VAL:HG12	1.94	0.49
2:A:384:ILE:O	2:A:388:ARG:HG2	2.13	0.49
2:A:264:LYS:O	2:A:268:GLY:HA2	2.12	0.48
1:B:34:C:O2	2:A:426:LEU:HB3	2.13	0.48
2:A:188:ASN:HD21	2:A:231:LYS:HE2	1.76	0.48
2:A:466:LEU:O	2:A:467:SER:C	2.51	0.48
2:A:465:LYS:CD	2:A:465:LYS:N	2.63	0.48
1:B:38:A:C2'	1:B:39:U:H5'	2.43	0.48
1:B:55:U:O2	1:B:57:G:C8	2.67	0.48
2:A:196:THR:HB	2:A:199:GLU:HB3	1.95	0.48
2:A:321:ARG:NH1	2:A:332:PRO:O	2.46	0.48
2:A:121:GLU:HB2	2:A:128:PRO:HD3	1.95	0.48
1:B:47:U:N3	1:B:48:U:C5	2.82	0.47
2:A:420:TYR:CD1	2:A:430:LEU:HD12	2.48	0.47
1:B:33:U:O2'	2:A:382:ASP:O	2.31	0.47
1:B:34:C:C2	2:A:426:LEU:HB3	2.49	0.47
2:A:224:ALA:O	2:A:448:ARG:NE	2.47	0.47
1:B:33:U:C2	1:B:35:C:OP2	2.67	0.47
1:B:38:A:H2'	1:B:39:U:H5'	1.96	0.47
2:A:102:LYS:NZ	2:A:105:VAL:CG1	2.76	0.47
2:A:102:LYS:HZ2	2:A:105:VAL:HG13	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:228:ASP:OD2	2:A:231:LYS:HE3	2.15	0.47
2:A:319:MET:O	2:A:323:VAL:HG13	2.15	0.47
2:A:199:GLU:HB2	2:A:280:PHE:CE1	2.50	0.47
2:A:425:MET:HG3	2:A:429:GLU:CG	2.45	0.47
2:A:124:THR:HB	2:A:186:VAL:HG13	1.96	0.47
2:A:407:LEU:HD23	2:A:413:LEU:HA	1.97	0.46
1:B:58:A:O2'	1:B:59:A:P	2.73	0.46
2:A:299:ASP:OD1	2:A:299:ASP:O	2.33	0.46
1:B:29:U:H2'	1:B:30:G:H8	1.80	0.46
2:A:119:ARG:HB3	2:A:147:LEU:HD13	1.97	0.46
1:B:26:G:H2'	1:B:27:U:H6	1.80	0.46
2:A:420:TYR:CE1	2:A:430:LEU:HD12	2.50	0.46
1:B:61:C:H2'	1:B:62:A:C8	2.51	0.46
1:B:26:G:O2'	1:B:27:U:H5'	2.16	0.46
2:A:373:ASN:HA	2:A:431:LYS:HE2	1.98	0.45
1:B:25:C:C2'	1:B:26:G:H5'	2.46	0.45
1:B:32:C:H2'	1:B:33:U:C5'	2.29	0.45
1:B:34:C:H5'	1:B:35:C:OP2	2.16	0.45
2:A:300:ARG:HG2	2:A:300:ARG:HH11	1.79	0.45
2:A:333:ALA:C	2:A:334:LEU:HD12	2.37	0.45
2:A:260:PHE:O	2:A:263:VAL:HG23	2.16	0.45
1:B:52:U:H2'	1:B:53:G:O4'	2.16	0.45
1:B:74:C:O3'	1:B:75:C:O4'	2.34	0.45
2:A:295:GLN:OE1	2:A:295:GLN:N	2.45	0.45
2:A:314:ASP:OD1	2:A:336:HIS:HE1	2.00	0.45
1:B:74:C:O2'	1:B:75:C:O5'	2.35	0.45
1:B:6:C:H2'	1:B:7:G:O4'	2.17	0.45
2:A:124:THR:HG21	2:A:186:VAL:CG1	2.47	0.45
2:A:219:ALA:O	2:A:223:ILE:HG13	2.17	0.45
2:A:207:THR:CG2	2:A:210:GLN:H	2.29	0.44
2:A:343:LEU:HA	2:A:398:VAL:HG11	1.99	0.44
2:A:280:PHE:N	2:A:281:PRO:CD	2.80	0.44
2:A:200:LYS:HD3	2:A:200:LYS:HA	1.80	0.44
1:B:29:U:H2'	1:B:30:G:C8	2.52	0.44
1:B:5:U:H2'	1:B:6:C:C6	2.53	0.44
2:A:266:ILE:HD13	2:A:319:MET:HB2	2.00	0.43
1:B:35:C:O2'	2:A:373:ASN:O	2.36	0.43
1:B:23:C:C2'	1:B:24:G:H5''	2.49	0.43
2:A:141:ARG:HB2	2:A:334:LEU:HB2	2.01	0.43
1:B:58:A:O2'	1:B:59:A:OP1	2.37	0.43
2:A:364:THR:HG23	2:A:367:GLN:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:102:LYS:HA	2:A:105:VAL:CG1	2.49	0.43
2:A:229:ILE:HG23	2:A:230:ASN:N	2.33	0.43
2:A:100:TYR:OH	2:A:339:PHE:HD2	2.01	0.43
2:A:361:LEU:HD13	2:A:445:HIS:CE1	2.54	0.43
2:A:362:THR:HA	2:A:446:GLN:NE2	2.33	0.43
1:B:58:A:C2'	1:B:59:A:O5'	2.66	0.42
2:A:191:LEU:HD21	2:A:193:ILE:HD11	2.02	0.42
1:B:28:C:H2'	1:B:29:U:H6	1.81	0.42
1:B:65:U:H2'	1:B:66:C:C6	2.53	0.42
2:A:102:LYS:HZ2	2:A:105:VAL:CG1	2.33	0.42
2:A:207:THR:HG23	2:A:210:GLN:H	1.84	0.42
2:A:238:LEU:HD12	2:A:238:LEU:HA	1.80	0.42
1:B:8:U:C4	1:B:13:C:H5	2.37	0.42
2:A:102:LYS:HD2	2:A:105:VAL:HG11	2.01	0.42
2:A:129:HIS:HB2	2:A:182:TRP:CD2	2.54	0.42
2:A:184:GLN:NE2	2:A:228:ASP:H	2.18	0.42
2:A:102:LYS:HA	2:A:102:LYS:HD2	1.70	0.42
2:A:350:MET:HB2	2:A:357:SER:OG	2.19	0.42
1:B:6:C:O2'	1:B:7:G:H5'	2.20	0.41
2:A:192:VAL:HG11	2:A:293:PHE:CZ	2.55	0.41
2:A:381:ARG:CG	2:A:387:HIS:HA	2.50	0.41
2:A:204:LYS:HA	2:A:204:LYS:NZ	2.34	0.41
2:A:444:GLU:O	2:A:447:ALA:HB3	2.20	0.41
2:A:229:ILE:CG2	2:A:230:ASN:N	2.83	0.41
2:A:139:SER:HB3	2:A:336:HIS:CD2	2.55	0.41
2:A:409:ASP:OD2	2:A:412:LYS:HG3	2.21	0.41
1:B:70:G:O2'	1:B:71:U:H5'	2.21	0.41
1:B:23:C:N3	1:B:25:C:N4	2.69	0.41
2:A:124:THR:CB	2:A:186:VAL:HG13	2.50	0.41
2:A:288:SER:OG	2:A:307:ILE:HD11	2.21	0.41
1:B:43:A:H2'	1:B:44:A:H8	1.85	0.41
2:A:240:TYR:CE1	2:A:244:SER:HB2	2.56	0.41
2:A:314:ASP:OD1	2:A:336:HIS:CE1	2.74	0.41
1:B:8:U:N3	1:B:13:C:H5	2.19	0.40
2:A:114:LYS:HA	2:A:114:LYS:HD2	1.67	0.40
2:A:270:THR:C	2:A:272:SER:N	2.74	0.40
2:A:184:GLN:HE22	2:A:228:ASP:H	1.70	0.40
2:A:197:ASP:HB3	2:A:215:ALA:HB2	2.04	0.40
2:A:317:PHE:HB2	2:A:334:LEU:HD21	2.04	0.40
1:B:32:C:C3'	1:B:33:U:C5'	2.99	0.40
2:A:457:VAL:HG12	2:A:461:MET:HE3	2.04	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	371/384 (97%)	348 (94%)	21 (6%)	2 (0%)	29 68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	467	SER
2	A	382	ASP

### 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	330/340 (97%)	299 (91%)	31 (9%)	8 32

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	103	LEU
2	A	114	LYS
2	A	115	GLU
2	A	156	PHE
2	A	159	TYR
2	A	171	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	A	174	LEU
2	A	202	LEU
2	A	203	TRP
2	A	204	LYS
2	A	232	THR
2	A	238	LEU
2	A	271	ASP
2	A	272	SER
2	A	296	ILE
2	A	300	ARG
2	A	323	VAL
2	A	347	GLN
2	A	351	SER
2	A	354	ASP
2	A	362	THR
2	A	384	ILE
2	A	404	THR
2	A	427	THR
2	A	429	GLU
2	A	441	LEU
2	A	444	GLU
2	A	464	ARG
2	A	465	LYS
2	A	468	PHE
2	A	469	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	A	140	HIS
2	A	145	GLN
2	A	170	HIS
2	A	188	ASN
2	A	257	HIS
2	A	262	GLN
2	A	284	GLN
2	A	336	HIS
2	A	373	ASN
2	A	389	GLN
2	A	445	HIS
2	A	446	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	74/75 (98%)	18 (24%)	2 (2%)

All (18) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	8	U
1	B	10	G
1	B	15	A
1	B	16	U
1	B	18	G
1	B	19	G
1	B	23	C
1	B	24	G
1	B	33	U
1	B	34	C
1	B	46	G
1	B	47	U
1	B	49	G
1	B	56	C
1	B	59	A
1	B	74	C
1	B	75	C
1	B	76	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	16	U
1	B	58	A

## 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

2 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	TRP	A	479	-	14,16,16	2.10	4 (28%)	16,22,22	0.94	0
3	SO4	A	478	-	4,4,4	0.30	0	6,6,6	0.06	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	TRP	A	479	-	-	1/7/8/8	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	479	TRP	OXT-C	5.87	1.49	1.30
4	A	479	TRP	CH2-CZ3	2.67	1.45	1.38
4	A	479	TRP	CZ3-CE3	2.56	1.42	1.36
4	A	479	TRP	CH2-CZ2	2.38	1.42	1.36

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	479	TRP	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	B	75/75 (100%)	4.03	61 (81%) 0 0	65, 132, 190, 198	0
2	A	373/384 (97%)	0.09	2 (0%) 91 75	27, 43, 73, 104	0
All	All	448/459 (97%)	0.75	63 (14%) 2 1	27, 47, 154, 198	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	9	G	11.2
1	B	24	G	10.5
1	B	19	G	9.8
1	B	18	G	8.6
1	B	46	G	8.4
1	B	55	U	7.9
1	B	73	A	7.7
1	B	57	G	7.6
1	B	20	U	7.5
1	B	16	U	7.5
1	B	47	U	7.4
1	B	23	C	7.3
1	B	56	C	7.2
1	B	45	G	7.0
1	B	41	A	7.0
1	B	42	G	6.6
1	B	54	U	6.0
1	B	21	A	6.0
1	B	8	U	5.5
1	B	74	C	5.3
1	B	69	G	5.2
1	B	76	A	5.1
1	B	25	C	4.6
1	B	53	G	4.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	13	C	4.4
1	B	30	G	4.3
1	B	75	C	4.3
1	B	44	A	4.2
1	B	22	G	4.1
1	B	43	A	4.0
1	B	58	A	3.6
1	B	10	G	3.6
1	B	12	G	3.5
1	B	70	G	3.4
1	B	71	U	3.3
1	B	61	C	3.3
1	B	51	G	3.3
1	B	40	C	3.3
1	B	1	G	3.3
1	B	48	U	3.3
1	B	72	C	3.3
1	B	31	A	3.2
1	B	32	C	3.1
2	A	469	ASP	3.1
1	B	4	C	3.1
1	B	63	C	2.8
1	B	60	U	2.8
1	B	29	U	2.7
1	B	27	U	2.7
1	B	14	A	2.6
1	B	33	U	2.5
1	B	15	A	2.5
1	B	64	G	2.4
1	B	3	C	2.3
1	B	5	U	2.3
1	B	52	U	2.2
1	B	26	G	2.2
2	A	382	ASP	2.2
1	B	7	G	2.2
1	B	62	A	2.1
1	B	34	C	2.1
1	B	50	C	2.0
1	B	49	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 monosaccharides 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
4	TRP	A	479	15/15	0.95	0.32	32,35,55,66	0
3	SO4	A	478	5/5	0.96	0.26	83,83,84,84	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.