



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 09:49 AM BST

PDB ID : 1EVK  
Title : CRYSTAL STRUCTURE OF A TRUNCATED FORM OF THREONYL-TRNA SYNTHETASE WITH THE LIGAND THREONINE  
Authors : Sankaranarayanan, R.; Dock-Bregeon, A.C.; Rees, B.; Moras, D.  
Deposited on : 2000-04-20  
Resolution : 2.00 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 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 : 2.14.4.dev1  
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) : 2.14.4.dev1

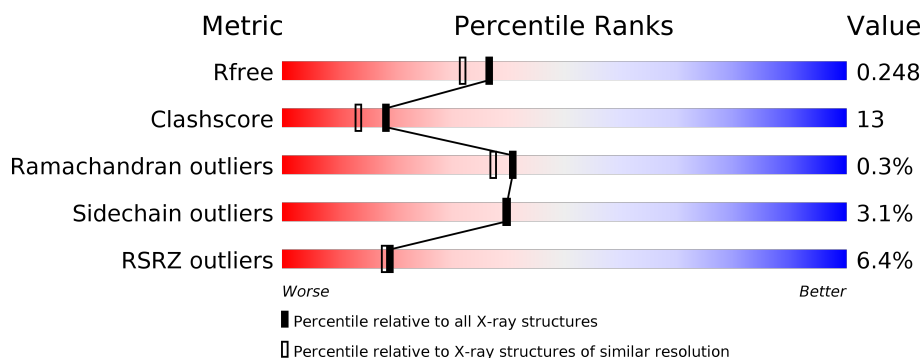
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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	A	401	<div> <div>10%</div> <div> <div></div> <div>73%</div> <div>25%</div> </div> </div>
1	B	401	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>20%</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7034 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.

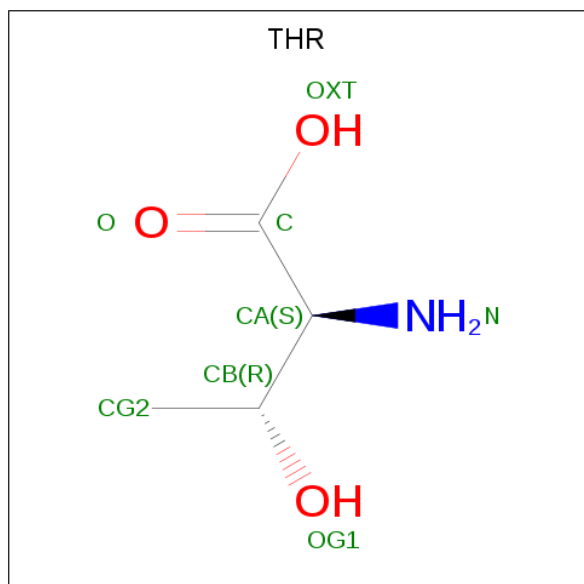
- Molecule 1 is a protein called THREONYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3273	2066	576	608	23			
1	B	401	Total	C	N	O	S	0	0	0
			3273	2066	576	608	23			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is THREONINE (three-letter code: THR) (formula: C<sub>4</sub>H<sub>9</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			8	4	1	3		

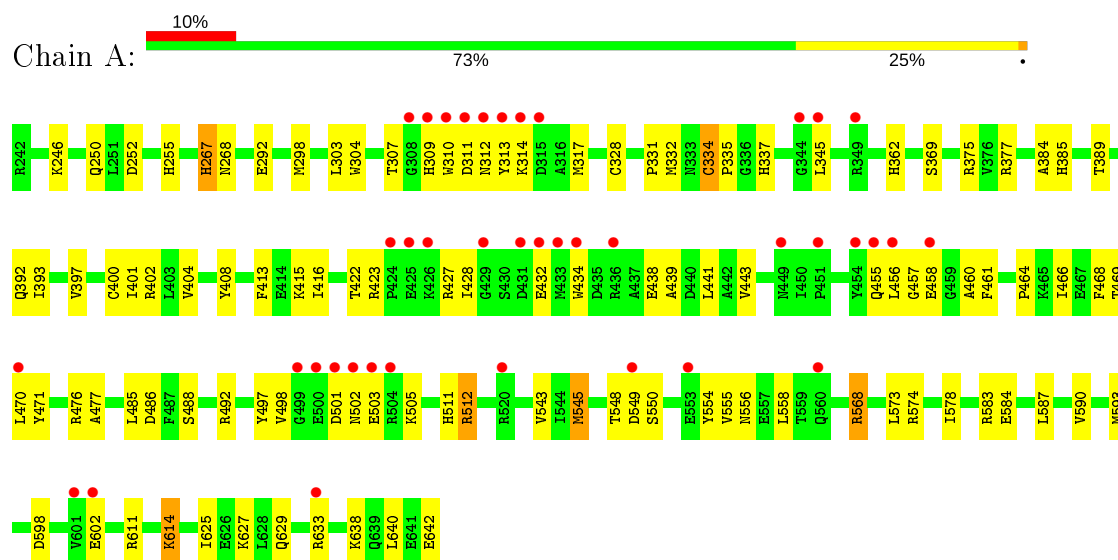
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	200	Total	O	0	0
			200	200		
4	B	278	Total	O	0	0
			278	278		

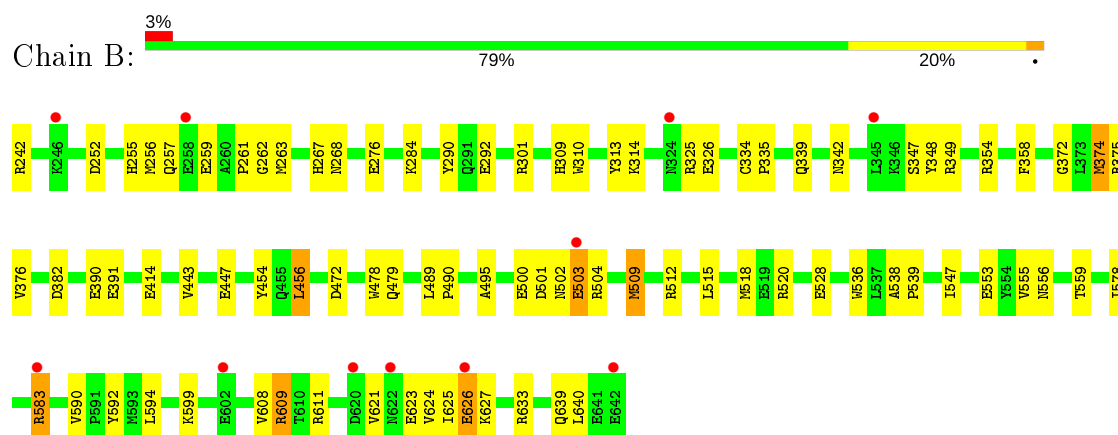
### 3 Residue-property plots

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 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: THREONYL-TRNA SYNTHETASE



#### • Molecule 1: THREONYL-TRNA SYNTHETASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.05Å 117.34Å 87.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.00 10.97 – 2.00	Depositor EDS
% Data completeness (in resolution range)	89.1 (12.00-2.00) 93.1 (10.97-2.00)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.212 , 0.241 0.219 , 0.248	Depositor DCC
$R_{free}$ test set	3737 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.6	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.49 , 76.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7034	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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: ZN

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	A	0.40	0/3344	0.64	1/4501 (0.0%)
1	B	0.44	0/3344	0.66	1/4501 (0.0%)
All	All	0.42	0/6688	0.65	2/9002 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	568	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	B	358	PHE	N-CA-C	-5.34	96.58	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3273	0	3203	103	0
1	B	3273	0	3203	76	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	B	8	0	6	0	0
4	A	200	0	0	2	0
4	B	278	0	0	9	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7034	0	6412	173	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 13.

All (173) 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:609:ARG:HH11	1:B:609:ARG:HB3	1.29	0.97
1:A:598:ASP:O	1:A:602:GLU:HG2	1.70	0.89
1:A:309:HIS:CE1	1:A:331:PRO:HG3	2.12	0.85
1:A:334:CYS:HB2	1:A:335:PRO:HD3	1.63	0.78
1:B:609:ARG:NH1	1:B:609:ARG:HB3	1.98	0.77
1:B:583:ARG:HG2	1:B:583:ARG:HH11	1.49	0.77
1:A:268:ASN:HD22	1:B:292:GLU:H	1.32	0.76
1:A:545:MET:CE	1:A:593:MET:HB3	2.16	0.76
1:A:554:TYR:O	1:A:558:LEU:HD13	1.87	0.74
1:B:257:GLN:HE21	1:B:259:GLU:CG	2.00	0.74
1:A:413:PHE:HB3	1:A:470:LEU:HD22	1.69	0.74
1:A:255:HIS:ND1	1:A:267:HIS:HE1	1.86	0.72
1:B:255:HIS:ND1	1:B:267:HIS:HE1	1.88	0.71
1:A:455:GLN:HB3	1:A:458:GLU:OE1	1.91	0.70
1:A:400:CYS:O	1:A:404:VAL:HG23	1.93	0.68
1:B:325:ARG:HD3	4:B:867:HOH:O	1.91	0.68
1:A:415:LYS:C	1:A:416:ILE:HD12	2.14	0.68
1:B:501:ASP:OD1	1:B:503:GLU:HB3	1.94	0.67
1:A:309:HIS:CE1	1:A:313:TYR:HB2	2.30	0.67
1:B:621:VAL:O	1:B:624:VAL:HG22	1.94	0.66
1:B:490:PRO:HD3	1:B:509:MET:HE3	1.78	0.66
1:A:428:ILE:HG12	1:A:461:PHE:HD1	1.61	0.65
1:B:252:ASP:OD1	1:B:267:HIS:HD2	1.79	0.65
1:A:303:LEU:HD12	1:B:259:GLU:HG3	1.78	0.65
1:A:309:HIS:NE2	1:A:331:PRO:HG3	2.12	0.64
1:B:242:ARG:N	4:B:984:HOH:O	2.31	0.64
1:A:310:TRP:O	1:A:314:LYS:HB2	1.99	0.62
1:A:501:ASP:O	1:A:503:GLU:N	2.33	0.62
1:A:309:HIS:NE2	1:A:331:PRO:CG	2.63	0.61
1:A:304:TRP:HZ3	1:A:332:MET:HE2	1.65	0.61
1:A:252:ASP:OD1	1:A:267:HIS:HD2	1.84	0.60
1:A:408:TYR:CD2	1:A:470:LEU:HD21	2.36	0.60
1:A:583:ARG:HB3	1:A:583:ARG:HH11	1.66	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:555:VAL:O	1:B:559:THR:HG22	2.02	0.60
1:A:625:ILE:O	1:A:629:GLN:HG3	2.02	0.60
1:B:390:GLU:CD	1:B:390:GLU:H	2.05	0.60
1:B:348:TYR:OH	1:B:349:ARG:NH1	2.35	0.59
1:A:413:PHE:CB	1:A:470:LEU:HD22	2.31	0.59
1:B:627:LYS:HB3	1:B:640:LEU:HD21	1.85	0.59
1:A:638:LYS:HB3	1:A:642:GLU:HG3	1.84	0.59
1:A:397:VAL:O	1:A:401:ILE:HG12	2.02	0.58
1:A:309:HIS:CE1	1:A:313:TYR:CB	2.87	0.58
1:B:242:ARG:N	4:B:993:HOH:O	2.36	0.58
1:A:427:ARG:HD2	1:A:434:TRP:NE1	2.18	0.58
1:B:583:ARG:HG2	1:B:583:ARG:NH1	2.17	0.58
1:B:609:ARG:CB	1:B:609:ARG:HH11	2.12	0.58
1:B:276:GLU:HG2	1:B:536:TRP:O	2.03	0.58
1:A:389:THR:HG22	1:A:497:TYR:OH	2.05	0.57
1:A:464:PRO:HG2	1:A:485:LEU:HD12	1.87	0.57
1:A:369:SER:HB2	1:A:375:ARG:NH2	2.20	0.56
1:A:310:TRP:HZ3	1:A:328:CYS:SG	2.28	0.56
1:A:568:ARG:NH2	4:A:720:HOH:O	2.39	0.55
1:B:348:TYR:CE2	1:B:500:GLU:HG2	2.42	0.55
1:B:590:VAL:O	1:B:611:ARG:HB3	2.07	0.55
1:B:559:THR:HG23	4:B:943:HOH:O	2.06	0.55
1:A:310:TRP:O	1:A:314:LYS:CB	2.55	0.54
1:A:548:THR:C	1:A:550:SER:H	2.09	0.54
1:A:423:ARG:O	1:A:457:GLY:HA2	2.07	0.54
1:A:334:CYS:HB2	1:A:335:PRO:CD	2.37	0.54
1:A:309:HIS:HE2	1:A:331:PRO:CG	2.21	0.53
1:A:389:THR:OG1	1:A:392:GLN:HG3	2.08	0.53
1:B:515:LEU:HD12	1:B:518:MET:CE	2.38	0.53
1:B:547:ILE:HD13	1:B:578:ILE:HD13	1.90	0.53
1:B:257:GLN:HG3	1:B:259:GLU:HG2	1.90	0.53
1:A:423:ARG:HA	1:A:434:TRP:CZ3	2.45	0.53
1:A:633:ARG:HG2	1:A:633:ARG:HH11	1.73	0.52
1:A:309:HIS:HD2	1:A:332:MET:SD	2.32	0.52
1:B:515:LEU:HD12	1:B:518:MET:HE1	1.92	0.52
1:A:255:HIS:ND1	1:A:267:HIS:CE1	2.75	0.51
1:A:334:CYS:CB	1:A:335:PRO:HD3	2.35	0.51
1:A:416:ILE:N	1:A:416:ILE:HD12	2.25	0.51
1:A:455:GLN:O	1:A:458:GLU:HB2	2.11	0.51
1:A:486:ASP:HB2	1:A:511:HIS:NE2	2.26	0.51
1:A:303:LEU:HD23	1:A:303:LEU:O	2.10	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:GLN:O	1:B:520:ARG:NH1	2.39	0.50
1:A:304:TRP:CZ3	1:A:332:MET:HE2	2.45	0.50
1:A:408:TYR:CG	1:A:470:LEU:HD21	2.47	0.50
1:B:490:PRO:HD3	1:B:509:MET:CE	2.40	0.50
1:A:292:GLU:H	1:B:268:ASN:HD22	1.59	0.50
1:A:310:TRP:CE3	1:A:317:MET:HE3	2.46	0.50
1:B:443:VAL:O	1:B:447:GLU:HG3	2.12	0.50
1:A:555:VAL:HG11	1:A:573:LEU:HD21	1.94	0.49
1:B:255:HIS:ND1	1:B:267:HIS:CE1	2.75	0.49
1:B:310:TRP:CE2	1:B:314:LYS:HD3	2.47	0.49
1:B:594:LEU:HD22	1:B:608:VAL:HG22	1.94	0.49
1:A:298:MET:HG2	1:B:263:MET:HE1	1.95	0.48
1:B:257:GLN:HE21	1:B:259:GLU:HG3	1.77	0.48
1:B:348:TYR:CD2	1:B:500:GLU:HG2	2.49	0.48
1:B:490:PRO:HG2	4:B:958:HOH:O	2.12	0.48
1:B:301:ARG:NH1	1:B:326:GLU:OE1	2.43	0.48
1:B:261:PRO:HG2	4:B:893:HOH:O	2.13	0.48
1:A:498:VAL:HA	1:A:503:GLU:O	2.13	0.47
1:A:310:TRP:HZ3	1:A:328:CYS:HG	1.62	0.47
1:A:246:LYS:O	1:A:250:GLN:HG3	2.14	0.47
1:A:298:MET:HG2	1:B:263:MET:CE	2.45	0.47
1:B:624:VAL:HG23	1:B:625:ILE:N	2.29	0.47
1:A:471:TYR:HA	1:A:476:ARG:O	2.14	0.47
1:A:543:VAL:HG23	1:A:590:VAL:HG11	1.97	0.47
1:A:590:VAL:O	1:A:611:ARG:HB3	2.15	0.47
1:A:268:ASN:ND2	1:B:292:GLU:H	2.04	0.47
1:B:583:ARG:HD3	1:B:583:ARG:O	2.15	0.47
1:A:422:THR:HG22	1:A:438:GLU:OE1	2.15	0.46
1:A:428:ILE:CG1	1:A:461:PHE:HD1	2.27	0.46
1:B:257:GLN:HE21	1:B:259:GLU:HG2	1.76	0.46
1:B:342:ASN:HD21	1:B:495:ALA:HA	1.79	0.46
1:A:497:TYR:OH	1:A:505:LYS:HE3	2.15	0.46
1:A:614:LYS:HG2	4:A:801:HOH:O	2.15	0.46
1:B:623:GLU:HG3	1:B:627:LYS:HE2	1.97	0.46
1:B:256:MET:HE1	1:B:372:GLY:HA2	1.97	0.46
1:A:554:TYR:CE1	1:A:558:LEU:HD11	2.50	0.46
1:A:545:MET:HG3	1:A:578:ILE:HD11	1.98	0.46
1:A:583:ARG:NH1	1:A:583:ARG:HB3	2.30	0.46
1:A:633:ARG:HG2	1:A:633:ARG:NH1	2.30	0.46
1:B:382:ASP:HB3	1:B:518:MET:HE1	1.97	0.46
1:A:556:ASN:HD21	1:A:573:LEU:HD11	1.81	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:592:TYR:OH	1:B:639:GLN:HB3	2.15	0.46
1:A:337:HIS:ND1	1:A:385:HIS:ND1	2.57	0.46
1:A:434:TRP:HH2	1:A:460:ALA:O	1.98	0.46
1:A:309:HIS:NE2	1:A:331:PRO:HG2	2.30	0.46
1:A:471:TYR:CE2	1:A:477:ALA:HB2	2.51	0.45
1:A:574:ARG:NH1	1:A:584:GLU:OE1	2.44	0.45
1:A:545:MET:HE1	1:A:593:MET:HB3	1.96	0.45
1:B:310:TRP:O	1:B:314:LYS:HB2	2.17	0.45
1:A:402:ARG:HG3	1:A:402:ARG:HH11	1.80	0.45
1:B:633:ARG:NH1	4:B:949:HOH:O	2.49	0.45
1:A:309:HIS:HE2	1:A:331:PRO:HG2	1.81	0.45
1:A:441:LEU:HD22	1:A:466:ILE:HG13	1.99	0.45
1:B:489:LEU:N	1:B:490:PRO:HD2	2.32	0.45
1:A:471:TYR:CZ	1:A:477:ALA:HB2	2.51	0.44
1:A:369:SER:HB2	1:A:375:ARG:HH21	1.80	0.44
1:B:310:TRP:CZ2	1:B:314:LYS:HD3	2.53	0.44
1:B:284:LYS:HA	1:B:284:LYS:HD3	1.86	0.44
1:A:469:THR:CG2	1:A:477:ALA:HB1	2.48	0.44
1:B:504:ARG:NH2	4:B:884:HOH:O	2.50	0.44
1:A:439:ALA:O	1:A:443:VAL:HG23	2.18	0.44
1:A:455:GLN:OE1	1:A:458:GLU:OE1	2.36	0.44
1:B:454:TYR:HB3	1:B:456:LEU:HD13	2.00	0.44
1:B:348:TYR:CZ	1:B:500:GLU:HG2	2.53	0.43
1:A:501:ASP:C	1:A:503:GLU:H	2.21	0.43
1:A:309:HIS:CE1	1:A:317:MET:SD	3.11	0.43
1:B:553:GLU:HB3	4:B:955:HOH:O	2.17	0.43
1:B:556:ASN:O	1:B:559:THR:CG2	2.66	0.43
1:B:556:ASN:O	1:B:559:THR:HG23	2.19	0.43
1:A:307:THR:O	1:A:492:ARG:HD3	2.19	0.43
1:B:504:ARG:HG2	1:B:504:ARG:HH11	1.84	0.43
1:B:503:GLU:HG3	1:B:504:ARG:N	2.33	0.43
1:A:583:ARG:O	1:A:587:LEU:HG	2.19	0.43
1:A:369:SER:O	1:A:375:ARG:NE	2.52	0.42
1:B:335:PRO:O	1:B:339:GLN:HG2	2.19	0.42
1:A:548:THR:C	1:A:550:SER:N	2.73	0.42
1:A:422:THR:OG1	1:A:456:LEU:HA	2.19	0.42
1:B:626:GLU:HG3	1:B:627:LYS:N	2.34	0.42
1:B:500:GLU:C	1:B:502:ASN:H	2.23	0.42
1:A:313:TYR:O	1:A:314:LYS:C	2.58	0.42
1:B:472:ASP:HB2	1:B:528:GLU:OE1	2.20	0.42
1:B:290:TYR:CD2	1:B:354:ARG:HB3	2.55	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:HIS:ND1	1:A:313:TYR:HB2	2.34	0.41
1:B:556:ASN:HA	1:B:559:THR:CG2	2.50	0.41
1:B:623:GLU:O	1:B:627:LYS:HG3	2.20	0.41
1:B:374:MET:HE3	1:B:478:TRP:CH2	2.54	0.41
1:B:262:GLY:O	1:B:376:VAL:HB	2.20	0.41
1:A:309:HIS:O	1:A:313:TYR:HB2	2.21	0.41
1:A:555:VAL:CG1	1:A:573:LEU:HD21	2.50	0.41
1:A:501:ASP:C	1:A:503:GLU:N	2.75	0.40
1:B:309:HIS:O	1:B:313:TYR:N	2.54	0.40
1:A:432:GLU:H	1:A:432:GLU:HG2	1.71	0.40
1:A:393:ILE:O	1:A:397:VAL:HG23	2.22	0.40
1:B:391:GLU:H	1:B:391:GLU:CD	2.24	0.40
1:A:362:HIS:HA	1:A:377:ARG:O	2.22	0.40
1:A:401:ILE:HD13	1:A:468:PHE:HZ	1.86	0.40
1:A:627:LYS:HB3	1:A:640:LEU:HD11	2.04	0.40
1:A:384:ALA:HB3	1:A:512:ARG:HD3	2.02	0.40
1:B:538:ALA:HA	1:B:539:PRO:HD3	1.97	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	
1	A	399/401 (100%)	381 (96%)	16 (4%)	2 (0%)	29	23
1	B	399/401 (100%)	388 (97%)	11 (3%)	0	100	100
All	All	798/802 (100%)	769 (96%)	27 (3%)	2 (0%)	41	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	502	ASN

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	549	ASP

### 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	
1	A	355/356 (100%)	346 (98%)	9 (2%)	47	49
1	B	355/356 (100%)	342 (96%)	13 (4%)	34	32
All	All	710/712 (100%)	688 (97%)	22 (3%)	40	40

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	267	HIS
1	A	311	ASP
1	A	312	ASN
1	A	334	CYS
1	A	345	LEU
1	A	488	SER
1	A	512	ARG
1	A	545	MET
1	A	614	LYS
1	B	334	CYS
1	B	347	SER
1	B	374	MET
1	B	375	ARG
1	B	414	GLU
1	B	456	LEU
1	B	503	GLU
1	B	509	MET
1	B	512	ARG
1	B	583	ARG
1	B	599	LYS
1	B	609	ARG
1	B	626	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	HIS
1	A	268	ASN
1	A	291	GLN
1	A	342	ASN
1	A	343	GLN
1	A	371	HIS
1	A	455	GLN
1	A	556	ASN
1	B	257	GLN
1	B	267	HIS
1	B	268	ASN
1	B	289	GLN
1	B	291	GLN
1	B	312	ASN
1	B	342	ASN
1	B	381	GLN
1	B	455	GLN
1	B	556	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 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 ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	THR	B	801	2	4,7,7	0.49	0	4,9,9	0.64	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	THR	B	801	2	-	0/4/8/8	-

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.

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	A	401/401 (100%)	0.32	40 (9%) 7 6	18, 39, 66, 77	0
1	B	401/401 (100%)	-0.15	11 (2%) 54 53	17, 32, 51, 67	0
All	All	802/802 (100%)	0.09	51 (6%) 19 18	17, 35, 61, 77	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	309	HIS	10.2
1	A	308	GLY	7.1
1	A	345	LEU	6.1
1	A	501	ASP	4.6
1	A	313	TYR	4.4
1	B	642	GLU	4.3
1	A	310	TRP	4.0
1	A	426	LYS	3.9
1	A	500	GLU	3.8
1	A	436	ARG	3.5
1	A	425	GLU	3.5
1	B	602	GLU	3.2
1	A	449	ASN	3.2
1	A	549	ASP	3.2
1	A	434	TRP	3.1
1	A	432	GLU	3.0
1	A	503	GLU	3.0
1	A	456	LEU	3.0
1	A	433	MET	2.9
1	A	349	ARG	2.8
1	A	311	ASP	2.8
1	A	502	ASN	2.8
1	A	455	GLN	2.7
1	A	344	GLY	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	431	ASP	2.7
1	A	504	ARG	2.6
1	B	345	LEU	2.6
1	B	324	ASN	2.6
1	B	503	GLU	2.5
1	B	246	LYS	2.5
1	A	429	GLY	2.5
1	B	583	ARG	2.4
1	A	314	LYS	2.4
1	A	451	PRO	2.4
1	A	553	GLU	2.3
1	A	602	GLU	2.3
1	B	258	GLU	2.3
1	A	454	TYR	2.3
1	A	424	PRO	2.2
1	A	470	LEU	2.2
1	B	622	ASN	2.2
1	B	626	GLU	2.2
1	A	458	GLU	2.2
1	A	633	ARG	2.1
1	A	499	GLY	2.1
1	A	312	ASN	2.1
1	A	601	VAL	2.1
1	A	315	ASP	2.0
1	A	560	GLN	2.0
1	A	520	ARG	2.0
1	B	620	ASP	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( $\text{\AA}^2$ )	Q<0.9
3	THR	B	801	8/8	0.95	0.09	21,22,24,24	0
2	ZN	A	1	1/1	0.96	0.06	40,40,40,40	0
2	ZN	B	2	1/1	1.00	0.07	22,22,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.