



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 08:54 pm GMT

PDB ID : 4HWT  
Title : Crystal structure of human Threonyl-tRNA synthetase bound to a novel inhibitor  
Authors : Hilgers, M.T.  
Deposited on : 2012-11-08  
Resolution : 2.30 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.

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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
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

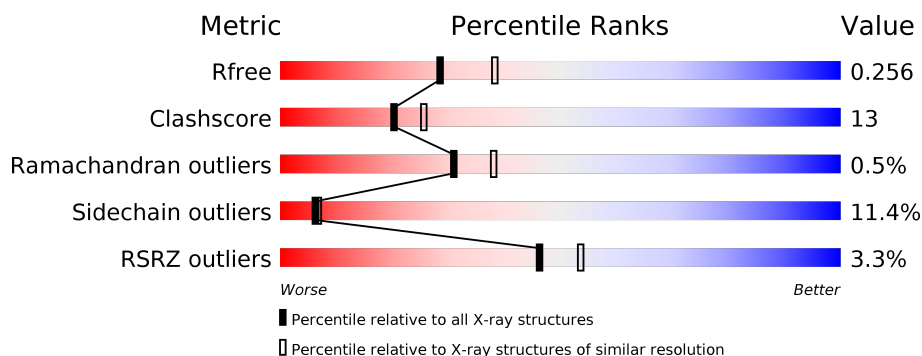
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	111664	4477 (2.30-2.30)
Clashscore	122126	5072 (2.30-2.30)
Ramachandran outliers	120053	5022 (2.30-2.30)
Sidechain outliers	120020	5021 (2.30-2.30)
RSRZ outliers	108989	4374 (2.30-2.30)

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.

Mol	Chain	Length	Quality of chain
1	A	413	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>20%</div> <div>• • •</div> </div> </div>
1	B	413	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>21%</div> <div>• • •</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6972 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 Threonine-tRNA ligase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			3258	2082	578	582	16			
1	B	402	Total	C	N	O	S	0	0	0
			3315	2113	587	599	16			

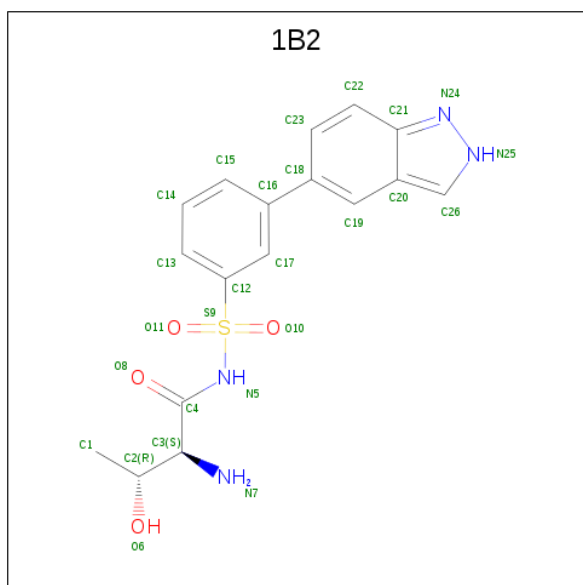
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	352	MET	-	EXPRESSION TAG	UNP P26639
A	353	ALA	-	EXPRESSION TAG	UNP P26639
A	757	LEU	-	EXPRESSION TAG	UNP P26639
A	758	GLU	-	EXPRESSION TAG	UNP P26639
A	759	HIS	-	EXPRESSION TAG	UNP P26639
A	760	HIS	-	EXPRESSION TAG	UNP P26639
A	761	HIS	-	EXPRESSION TAG	UNP P26639
A	762	HIS	-	EXPRESSION TAG	UNP P26639
A	763	HIS	-	EXPRESSION TAG	UNP P26639
A	764	HIS	-	EXPRESSION TAG	UNP P26639
B	352	MET	-	EXPRESSION TAG	UNP P26639
B	353	ALA	-	EXPRESSION TAG	UNP P26639
B	757	LEU	-	EXPRESSION TAG	UNP P26639
B	758	GLU	-	EXPRESSION TAG	UNP P26639
B	759	HIS	-	EXPRESSION TAG	UNP P26639
B	760	HIS	-	EXPRESSION TAG	UNP P26639
B	761	HIS	-	EXPRESSION TAG	UNP P26639
B	762	HIS	-	EXPRESSION TAG	UNP P26639
B	763	HIS	-	EXPRESSION TAG	UNP P26639
B	764	HIS	-	EXPRESSION TAG	UNP P26639

- 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 N-{[3-(2H-indazol-5-yl)phenyl]sulfonyl}-L-threoninamide (three-letter code: 1B2) (formula: C<sub>17</sub>H<sub>18</sub>N<sub>4</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	17	4	4	1		
3	B	1	Total	C	N	O	S	0	0
			26	17	4	4	1		

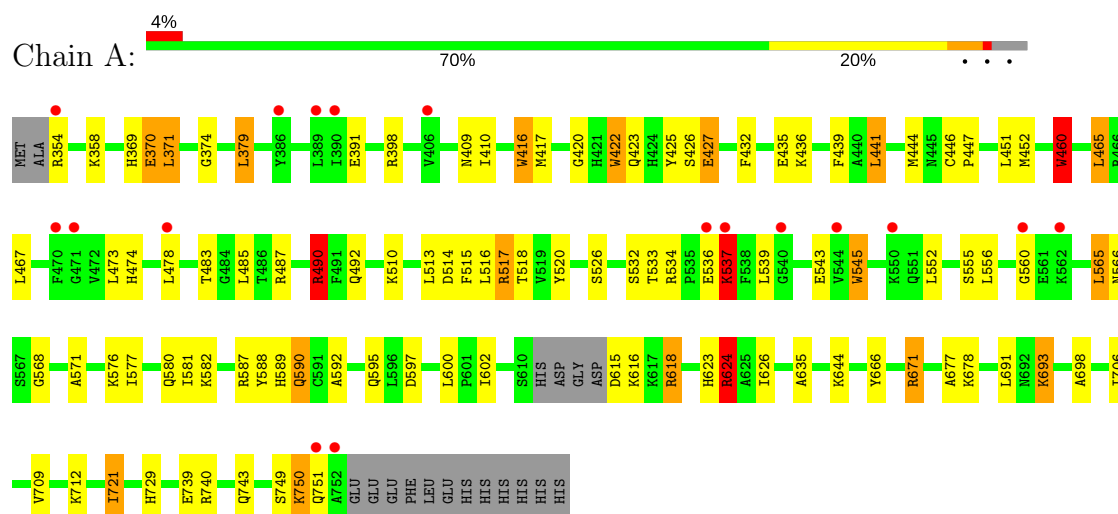
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	162	Total	O	0	0
			162	162		
4	B	183	Total	O	0	0
			183	183		

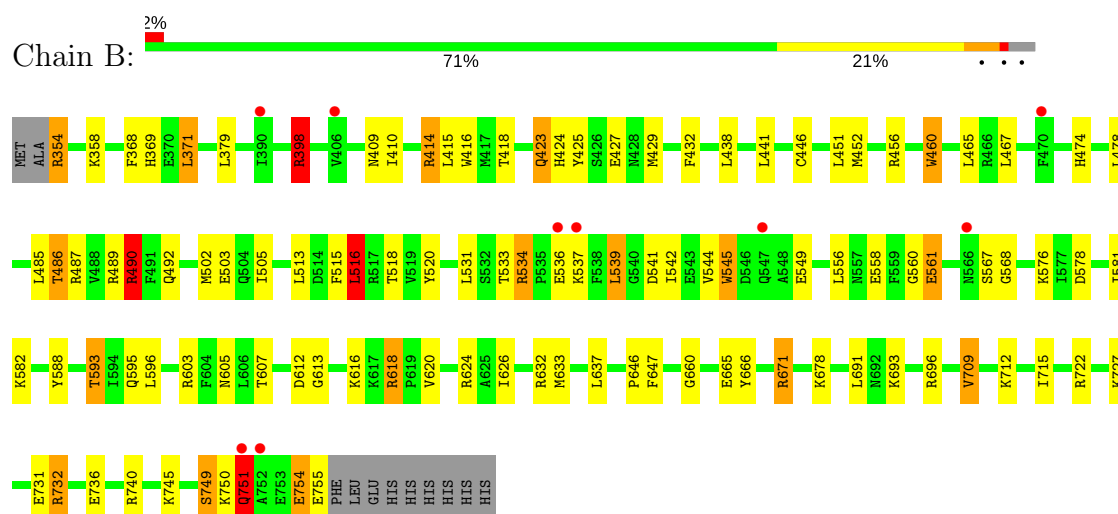
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Threonine-tRNA ligase, cytoplasmic



- Molecule 1: Threonine-tRNA ligase, cytoplasmic



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.90Å 73.90Å 357.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.19 – 2.30 42.19 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.8 (42.19-2.30) 97.8 (42.19-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.94 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.207 , 0.257 0.207 , 0.256	Depositor DCC
$R_{free}$ test set	2241 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.6	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 27.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6972	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1B2, 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	0.65	5/3338 (0.1%)	0.76	7/4498 (0.2%)
1	B	0.68	3/3397 (0.1%)	0.82	8/4579 (0.2%)
All	All	0.66	8/6735 (0.1%)	0.79	15/9077 (0.2%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	460	TRP	CD2-CE2	7.15	1.50	1.41
1	A	416	TRP	CD2-CE2	5.56	1.48	1.41
1	B	545	TRP	CD2-CE2	5.46	1.47	1.41
1	A	391	GLU	CD-OE1	5.32	1.31	1.25
1	A	545	TRP	CD2-CE2	5.28	1.47	1.41
1	A	460	TRP	CD2-CE2	5.25	1.47	1.41
1	B	416	TRP	CD2-CE2	5.06	1.47	1.41
1	A	422	TRP	CD2-CE2	5.03	1.47	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	624	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	B	539	LEU	CA-CB-CG	7.28	132.04	115.30
1	B	516	LEU	CA-CB-CG	6.98	131.36	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	490	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	B	398	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	B	671	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	490	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	B	490	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	B	751	GLN	N-CA-C	6.07	127.38	111.00
1	A	624	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	B	671	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	A	539	LEU	CA-CB-CG	5.80	128.63	115.30
1	A	441	LEU	CA-CB-CG	5.25	127.37	115.30
1	A	379	LEU	CA-CB-CG	5.24	127.35	115.30
1	A	465	LEU	CA-CB-CG	5.05	126.92	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	560	GLY	Peptide

## 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	A	3258	0	3206	91	0
1	B	3315	0	3243	95	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	26	0	18	5	0
3	B	26	0	17	0	0
4	A	162	0	0	35	0
4	B	183	0	0	35	0
All	All	6972	0	6484	175	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 (175) 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:A:721:ILE:HG21	4:A:971:HOH:O	1.23	1.26
1:A:410:ILE:HB	4:A:1032:HOH:O	1.46	1.15
1:B:503:GLU:HB2	4:B:1047:HOH:O	1.47	1.09
1:B:722:ARG:HB2	4:B:1061:HOH:O	1.55	1.07
1:A:526:SER:HB2	4:A:1019:HOH:O	1.62	1.00
1:A:452:MET:SD	4:B:1023:HOH:O	2.19	1.00
1:A:721:ILE:HG12	1:A:729:HIS:HB2	1.48	0.95
1:A:751:GLN:HA	4:A:1024:HOH:O	1.68	0.93
4:A:1043:HOH:O	1:B:452:MET:SD	2.28	0.90
1:B:745:LYS:HE3	4:B:1025:HOH:O	1.69	0.90
1:B:633:MET:HE3	1:B:637:LEU:HG	1.59	0.85
1:A:490:ARG:NH2	1:A:492:GLN:HE21	1.75	0.85
1:B:354:ARG:HH11	1:B:354:ARG:HG2	1.42	0.85
1:B:354:ARG:NH1	1:B:354:ARG:HG2	1.91	0.85
1:A:490:ARG:HH22	1:A:492:GLN:HE21	1.20	0.84
1:A:623:HIS:HB3	3:A:802:1B2:H4	1.60	0.84
1:B:646:PRO:HB3	1:B:750:LYS:HE3	1.59	0.83
1:B:558:GLU:HB3	4:B:1057:HOH:O	1.77	0.82
1:A:369:HIS:HE1	1:A:371:LEU:HD22	1.45	0.81
1:A:750:LYS:HE3	4:A:1027:HOH:O	1.80	0.80
1:B:456:ARG:HD2	4:B:1063:HOH:O	1.79	0.80
1:A:693:LYS:HE2	4:A:1046:HOH:O	1.81	0.80
1:B:354:ARG:HH11	1:B:354:ARG:CG	1.95	0.79
1:A:369:HIS:CE1	1:A:371:LEU:HD22	2.17	0.79
1:B:490:ARG:HH22	1:B:492:GLN:HE21	1.31	0.79
1:B:749:SER:HB2	4:B:1052:HOH:O	1.84	0.77
1:B:665:GLU:HG2	4:B:1068:HOH:O	1.85	0.77
1:B:544:VAL:HG23	4:B:1069:HOH:O	1.83	0.76
1:A:533:THR:CG2	4:A:998:HOH:O	2.34	0.76
1:B:516:LEU:HD22	1:B:520:TYR:CE2	2.22	0.75
1:B:516:LEU:CD2	1:B:520:TYR:CE2	2.69	0.75
1:B:647:PHE:HB2	1:B:751:GLN:HG2	1.68	0.74
1:A:444:MET:SD	3:A:802:1B2:N7	2.60	0.74
1:A:749:SER:HB3	4:A:977:HOH:O	1.87	0.73
1:A:409:ASN:HD22	1:B:490:ARG:HD2	1.53	0.73
1:A:555:SER:HB3	4:A:984:HOH:O	1.89	0.72
1:B:750:LYS:HB3	4:B:963:HOH:O	1.88	0.72
1:A:721:ILE:CG2	4:A:971:HOH:O	1.98	0.71
1:A:439:PHE:HB3	4:A:1032:HOH:O	1.91	0.70
1:B:502:MET:CE	4:B:962:HOH:O	2.38	0.70
1:B:418:THR:O	1:B:603:ARG:HD3	1.92	0.70
1:B:398:ARG:HG2	4:B:979:HOH:O	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:ARG:HH22	1:A:492:GLN:NE2	1.90	0.69
1:A:565:LEU:HD21	4:A:1040:HOH:O	1.93	0.69
1:A:624:ARG:HG3	1:A:624:ARG:HH11	1.57	0.69
1:B:516:LEU:HD21	1:B:520:TYR:HE2	1.58	0.68
1:A:422:TRP:HD1	4:A:1012:HOH:O	1.76	0.67
1:A:371:LEU:HD11	1:B:414:ARG:HG2	1.75	0.67
1:B:618:ARG:HD2	4:B:1044:HOH:O	1.94	0.67
1:B:536:GLU:O	1:B:537:LYS:HB2	1.95	0.67
1:A:534:ARG:HB3	1:A:545:TRP:CE3	2.30	0.66
1:A:552:LEU:O	1:A:556:LEU:HB2	1.95	0.66
1:A:490:ARG:HH11	1:B:409:ASN:HD21	1.42	0.66
1:A:533:THR:HB	1:A:568:GLY:H	1.60	0.66
1:B:750:LYS:HA	4:B:978:HOH:O	1.97	0.65
1:A:721:ILE:CG1	1:A:729:HIS:HB2	2.25	0.64
1:B:502:MET:HE1	4:B:962:HOH:O	1.96	0.64
1:B:633:MET:CE	1:B:637:LEU:HG	2.28	0.63
1:B:354:ARG:HB3	4:B:968:HOH:O	1.99	0.63
1:A:409:ASN:ND2	1:B:490:ARG:HD2	2.15	0.62
1:B:727:LYS:HD2	4:B:1054:HOH:O	1.97	0.62
1:B:490:ARG:NH2	1:B:492:GLN:HE21	1.94	0.62
1:A:358:LYS:HE2	4:A:968:HOH:O	2.01	0.60
1:B:369:HIS:CE1	1:B:371:LEU:HD22	2.36	0.60
1:B:516:LEU:HD21	1:B:520:TYR:CE2	2.36	0.60
1:B:722:ARG:CB	4:B:1061:HOH:O	2.27	0.60
1:B:740:ARG:HD3	1:B:754:GLU:O	2.01	0.60
1:B:505:ILE:HD11	1:B:620:VAL:HG21	1.84	0.59
1:A:409:ASN:HD21	1:B:490:ARG:HH11	1.49	0.59
1:A:624:ARG:O	1:A:624:ARG:HG3	2.03	0.59
1:B:727:LYS:HE2	4:B:960:HOH:O	2.01	0.59
1:A:422:TRP:O	1:A:426:SER:HB2	2.03	0.58
1:B:369:HIS:HE1	1:B:371:LEU:HD22	1.68	0.58
1:B:745:LYS:CE	4:B:1025:HOH:O	2.38	0.58
1:A:615:ASP:HB3	4:A:988:HOH:O	2.02	0.58
1:A:374:GLY:HA2	4:A:990:HOH:O	2.04	0.57
1:B:731:GLU:O	1:B:732:ARG:HG2	2.05	0.55
1:A:483:THR:HG22	4:A:1042:HOH:O	2.06	0.55
1:A:543:GLU:HG2	4:A:1023:HOH:O	2.06	0.55
1:A:602:ILE:HD13	1:A:618:ARG:HD3	1.88	0.55
1:A:427:GLU:H	1:A:427:GLU:CD	2.10	0.54
1:A:417:MET:HG2	4:A:1012:HOH:O	2.06	0.54
1:B:750:LYS:CB	4:B:963:HOH:O	2.49	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:HIS:CD2	1:B:410:ILE:HD12	2.43	0.54
1:A:534:ARG:HD2	4:A:986:HOH:O	2.08	0.53
1:A:582:LYS:HD2	4:A:1019:HOH:O	2.07	0.53
1:B:633:MET:HE2	1:B:637:LEU:HD21	1.91	0.53
1:B:474:HIS:NE2	1:B:490:ARG:HG3	2.24	0.53
1:B:605:ASN:OD1	1:B:618:ARG:NH2	2.42	0.53
1:B:732:ARG:HH11	1:B:732:ARG:CG	2.22	0.52
1:A:623:HIS:HB3	3:A:802:1B2:C1	2.34	0.52
1:A:698:ALA:CB	1:A:706:ILE:HD12	2.40	0.52
1:A:582:LYS:HB2	1:A:588:TYR:CE1	2.45	0.51
1:B:561:GLU:HG3	4:B:1050:HOH:O	2.09	0.51
1:A:536:GLU:O	1:A:537:LYS:HB3	2.11	0.51
1:A:520:TYR:OH	1:A:626:ILE:O	2.21	0.51
1:A:624:ARG:NH1	1:A:624:ARG:HG3	2.26	0.51
1:B:582:LYS:HB2	1:B:588:TYR:CE1	2.46	0.51
1:B:533:THR:HB	1:B:568:GLY:H	1.76	0.50
1:B:745:LYS:HD2	4:B:1025:HOH:O	2.10	0.50
1:A:452:MET:HE2	1:A:467:LEU:HD13	1.92	0.50
1:A:555:SER:CB	4:A:984:HOH:O	2.52	0.50
1:B:578:ASP:OD1	1:B:593:THR:CG2	2.59	0.50
1:A:420:GLY:HA2	1:A:423:GLN:NE2	2.27	0.50
1:A:666:TYR:HE2	1:A:709:VAL:HG22	1.77	0.50
1:B:486:THR:HB	4:B:1045:HOH:O	2.11	0.50
1:A:490:ARG:HH11	1:B:409:ASN:ND2	2.07	0.49
1:A:565:LEU:HD23	1:A:566:ASN:H	1.77	0.49
4:A:1010:HOH:O	1:B:371:LEU:HD13	2.13	0.49
1:B:666:TYR:HE1	1:B:709:VAL:HG22	1.77	0.49
1:A:533:THR:HG23	4:A:998:HOH:O	2.09	0.49
1:A:739:GLU:HG2	4:A:1011:HOH:O	2.13	0.49
1:A:616:LYS:HD2	4:A:989:HOH:O	2.12	0.49
1:B:520:TYR:CZ	1:B:581:ILE:HG21	2.48	0.49
1:A:532:SER:HB2	1:A:576:LYS:HB2	1.95	0.49
1:A:452:MET:HE3	1:B:379:LEU:HD23	1.95	0.48
1:A:398:ARG:HD2	1:B:678:LYS:HA	1.96	0.48
1:B:745:LYS:CD	4:B:1025:HOH:O	2.61	0.48
1:A:485:LEU:HB2	1:A:635:ALA:HB2	1.96	0.48
1:A:516:LEU:HD22	1:A:520:TYR:CE2	2.49	0.47
1:B:545:TRP:O	1:B:549:GLU:HG3	2.14	0.47
1:A:514:ASP:O	1:A:518:THR:HG23	2.15	0.47
1:A:416:TRP:CZ3	1:A:447:PRO:HG2	2.49	0.47
4:A:1043:HOH:O	1:B:452:MET:CE	2.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:576:LYS:HB3	1:B:595:GLN:HG2	1.97	0.46
1:B:607:THR:OG1	1:B:616:LYS:HE2	2.15	0.46
1:A:460:TRP:HZ2	4:A:996:HOH:O	1.95	0.46
1:A:409:ASN:ND2	1:B:490:ARG:HH11	2.12	0.46
1:B:693:LYS:HA	1:B:693:LYS:HD3	1.79	0.46
1:A:516:LEU:HD23	1:A:626:ILE:HG23	1.99	0.45
1:A:516:LEU:HD21	1:A:592:ALA:CB	2.47	0.45
1:A:432:PHE:HB3	1:B:432:PHE:HB3	1.98	0.44
1:B:660:GLY:HA3	4:B:1012:HOH:O	2.17	0.44
1:B:751:GLN:HG3	4:B:978:HOH:O	2.16	0.44
1:A:517:ARG:HG3	1:A:518:THR:N	2.32	0.44
1:B:474:HIS:HA	1:B:489:ARG:O	2.18	0.44
1:A:595:GLN:HE22	3:A:802:1B2:H10	1.64	0.44
1:A:534:ARG:NE	4:A:986:HOH:O	2.51	0.43
1:A:595:GLN:HB2	1:A:623:HIS:HB2	1.99	0.43
1:B:612:ASP:HA	1:B:613:GLY:HA2	1.82	0.43
1:A:545:TRP:HH2	1:A:571:ALA:O	2.00	0.43
1:B:423:GLN:HG2	1:B:424:HIS:CE1	2.53	0.43
1:B:537:LYS:CE	4:B:1055:HOH:O	2.66	0.43
1:B:581:ILE:O	1:B:588:TYR:HA	2.18	0.43
1:B:398:ARG:NH2	4:B:954:HOH:O	2.52	0.43
1:A:534:ARG:O	1:A:568:GLY:HA2	2.18	0.43
1:A:590:GLN:HB3	3:A:802:1B2:N25	2.33	0.43
1:B:368:PHE:HZ	1:B:485:LEU:HG	1.84	0.43
1:A:370:GLU:HG2	4:A:1045:HOH:O	2.18	0.43
1:A:526:SER:CB	4:A:1035:HOH:O	2.66	0.42
1:B:452:MET:HE2	1:B:467:LEU:HD13	2.01	0.42
1:B:633:MET:CE	1:B:637:LEU:CG	2.96	0.42
1:B:539:LEU:CD1	4:B:1031:HOH:O	2.67	0.42
1:B:425:TYR:HB3	1:B:429:MET:CE	2.49	0.42
1:B:490:ARG:HH22	1:B:492:GLN:NE2	2.08	0.42
1:B:732:ARG:NH1	1:B:732:ARG:CG	2.83	0.42
1:A:671:ARG:HD3	4:A:953:HOH:O	2.20	0.42
1:B:536:GLU:HA	1:B:536:GLU:OE1	2.20	0.42
1:B:418:THR:O	1:B:603:ARG:CD	2.66	0.41
1:B:755:GLU:HG2	4:B:1065:HOH:O	2.20	0.41
1:A:597:ASP:OD2	1:A:600:LEU:HB2	2.21	0.41
1:B:533:THR:HG23	4:B:1003:HOH:O	2.20	0.41
1:A:581:ILE:O	1:A:588:TYR:HA	2.20	0.41
1:A:677:ALA:N	1:A:678:LYS:HA	2.35	0.41
1:B:722:ARG:NE	4:B:1061:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:TYR:HD2	1:A:709:VAL:HG13	1.85	0.41
1:A:589:HIS:HA	4:A:1036:HOH:O	2.20	0.41
1:A:534:ARG:CD	4:A:986:HOH:O	2.69	0.41
1:A:698:ALA:HB1	1:A:706:ILE:HD12	2.02	0.41
1:B:534:ARG:HG2	1:B:549:GLU:OE2	2.21	0.40
1:A:698:ALA:HB3	1:A:706:ILE:HD12	2.02	0.40
1:B:534:ARG:HG3	4:B:1003:HOH:O	2.21	0.40
1:A:556:LEU:HD13	1:A:577:ILE:HD13	2.02	0.40
1:B:749:SER:OG	1:B:750:LYS:N	2.52	0.40
1:B:626:ILE:HD11	4:B:1006:HOH:O	2.21	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	
1	A	391/413 (95%)	377 (96%)	11 (3%)	3 (1%)	21	25
1	B	400/413 (97%)	384 (96%)	15 (4%)	1 (0%)	43	53
All	All	791/826 (96%)	761 (96%)	26 (3%)	4 (0%)	31	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	751	GLN
1	A	560	GLY
1	A	537	LYS
1	A	750	LYS

### 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	351/367 (96%)	315 (90%)	36 (10%)	8	9
1	B	357/367 (97%)	312 (87%)	45 (13%)	5	5
All	All	708/734 (96%)	627 (89%)	81 (11%)	6	7

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	354	ARG
1	A	370	GLU
1	A	371	LEU
1	A	379	LEU
1	A	425	TYR
1	A	427	GLU
1	A	435	GLU
1	A	436	LYS
1	A	441	LEU
1	A	446	CYS
1	A	451	LEU
1	A	460	TRP
1	A	465	LEU
1	A	473	LEU
1	A	478	LEU
1	A	487	ARG
1	A	490	ARG
1	A	510	LYS
1	A	513	LEU
1	A	515	PHE
1	A	517	ARG
1	A	537	LYS
1	A	565	LEU
1	A	580	GLN
1	A	587	ARG
1	A	590	GLN
1	A	618	ARG

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Mol	Chain	Res	Type
1	A	624	ARG
1	A	644	LYS
1	A	671	ARG
1	A	691	LEU
1	A	693	LYS
1	A	712	LYS
1	A	721	ILE
1	A	740	ARG
1	A	743	GLN
1	B	354	ARG
1	B	358	LYS
1	B	371	LEU
1	B	398	ARG
1	B	414	ARG
1	B	415	LEU
1	B	423	GLN
1	B	427	GLU
1	B	438	LEU
1	B	441	LEU
1	B	446	CYS
1	B	451	LEU
1	B	460	TRP
1	B	465	LEU
1	B	478	LEU
1	B	486	THR
1	B	487	ARG
1	B	490	ARG
1	B	513	LEU
1	B	515	PHE
1	B	516	LEU
1	B	518	THR
1	B	531	LEU
1	B	534	ARG
1	B	541	ASP
1	B	542	ILE
1	B	556	LEU
1	B	561	GLU
1	B	567	SER
1	B	593	THR
1	B	596	LEU
1	B	618	ARG
1	B	624	ARG

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Mol	Chain	Res	Type
1	B	632	ARG
1	B	671	ARG
1	B	691	LEU
1	B	696	ARG
1	B	709	VAL
1	B	712	LYS
1	B	715	ILE
1	B	732	ARG
1	B	736	GLU
1	B	749	SER
1	B	751	GLN
1	B	754	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	409	ASN
1	A	492	GLN
1	A	557	ASN
1	A	673	GLN
1	B	409	ASN
1	B	492	GLN
1	B	547	GLN
1	B	557	ASN
1	B	673	GLN

### 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 carbohydrates in this entry.



## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	1B2	A	802	2	24,28,28	2.55	2 (8%)	32,41,41	2.34	6 (18%)
3	1B2	B	802	2	24,28,28	2.40	2 (8%)	32,41,41	2.64	8 (25%)

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	1B2	A	802	2	-	0/23/23/23	0/3/3/3
3	1B2	B	802	2	-	0/23/23/23	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	1B2	C12-S9	-11.27	1.60	1.76
3	B	802	1B2	C12-S9	-10.68	1.61	1.76
3	B	802	1B2	N25-N24	2.81	1.42	1.37
3	A	802	1B2	N25-N24	3.01	1.43	1.37

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	1B2	O11-S9-O10	-11.01	105.72	119.56
3	A	802	1B2	O11-S9-O10	-9.75	107.31	119.56
3	B	802	1B2	C20-C26-N25	-3.19	103.19	111.32
3	A	802	1B2	C20-C26-N25	-3.01	103.66	111.32
3	B	802	1B2	C23-C18-C19	2.34	121.55	118.17
3	A	802	1B2	C26-C20-C21	2.90	110.81	104.66
3	A	802	1B2	C4-N5-S9	3.06	127.46	124.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	1B2	O11-S9-N5	3.08	115.50	106.75
3	B	802	1B2	C26-C20-C21	3.34	111.73	104.66
3	B	802	1B2	C4-N5-S9	3.38	127.79	124.21
3	A	802	1B2	C12-S9-N5	3.40	110.57	105.89
3	B	802	1B2	C12-S9-N5	3.53	110.75	105.89
3	A	802	1B2	C22-C21-N24	3.85	136.49	130.19
3	B	802	1B2	C22-C21-N24	3.96	136.67	130.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	1B2	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

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	395/413 (95%)	0.18	17 (4%) 35 42	28, 43, 79, 109	0
1	B	402/413 (97%)	0.06	9 (2%) 62 69	29, 39, 64, 93	0
All	All	797/826 (96%)	0.12	26 (3%) 46 53	28, 41, 73, 109	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	560	GLY	5.9
1	A	752	ALA	4.5
1	A	537	LYS	3.6
1	B	406	VAL	3.2
1	B	537	LYS	2.9
1	A	562	LYS	2.8
1	A	354	ARG	2.8
1	B	536	GLU	2.7
1	A	478	LEU	2.6
1	B	390	ILE	2.5
1	A	550	LYS	2.5
1	B	752	ALA	2.4
1	A	390	ILE	2.4
1	A	751	GLN	2.3
1	A	406	VAL	2.3
1	A	536	GLU	2.3
1	B	566	ASN	2.2
1	A	540	GLY	2.2
1	B	751	GLN	2.2
1	B	470	PHE	2.2
1	A	470	PHE	2.1
1	A	544	VAL	2.1
1	A	471	GLY	2.1
1	A	389	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	547	GLN	2.0
1	A	386	TYR	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 carbohydrates 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	1B2	B	802	26/26	0.93	0.17	46,54,60,62	0
3	1B2	A	802	26/26	0.94	0.19	59,68,98,103	0
2	ZN	B	801	1/1	0.99	0.09	40,40,40,40	0
2	ZN	A	801	1/1	0.99	0.08	49,49,49,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.