



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 09:38 AM GMT

PDB ID : 3KT8
Title : Crystal structure of *S. cerevisiae* tryptophanyl-tRNA synthetase in complex with L-tryptophanamide
Authors : Zhou, M.; Dong, X.; Zhong, C.; Shen, N.; Ding, J.
Deposited on : 2009-11-24
Resolution : 3.00 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

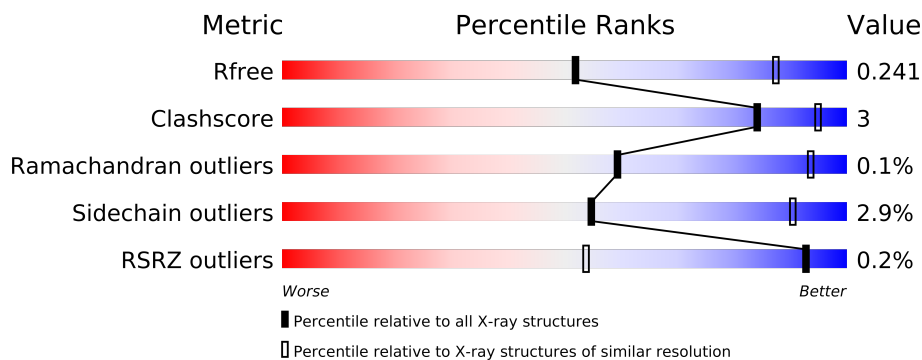
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	438	
1	B	438	
1	C	438	
1	D	438	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13222 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Tryptophanyl-tRNA synthetase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	0	0
			3287	2118	545	611	13			
1	B	403	Total	C	N	O	S	0	0	0
			3250	2096	539	602	13			
1	C	403	Total	C	N	O	S	0	0	0
			3250	2096	539	602	13			
1	D	410	Total	C	N	O	S	0	0	0
			3304	2129	547	615	13			

There are 24 discrepancies between the modelled and reference sequences:

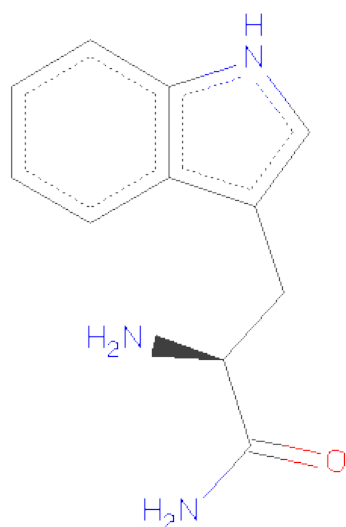
Chain	Residue	Modelled	Actual	Comment	Reference
A	433	HIS	-	EXPRESSION TAG	UNP Q12109
A	434	HIS	-	EXPRESSION TAG	UNP Q12109
A	435	HIS	-	EXPRESSION TAG	UNP Q12109
A	436	HIS	-	EXPRESSION TAG	UNP Q12109
A	437	HIS	-	EXPRESSION TAG	UNP Q12109
A	438	HIS	-	EXPRESSION TAG	UNP Q12109
B	433	HIS	-	EXPRESSION TAG	UNP Q12109
B	434	HIS	-	EXPRESSION TAG	UNP Q12109
B	435	HIS	-	EXPRESSION TAG	UNP Q12109
B	436	HIS	-	EXPRESSION TAG	UNP Q12109
B	437	HIS	-	EXPRESSION TAG	UNP Q12109
B	438	HIS	-	EXPRESSION TAG	UNP Q12109
C	433	HIS	-	EXPRESSION TAG	UNP Q12109
C	434	HIS	-	EXPRESSION TAG	UNP Q12109
C	435	HIS	-	EXPRESSION TAG	UNP Q12109
C	436	HIS	-	EXPRESSION TAG	UNP Q12109
C	437	HIS	-	EXPRESSION TAG	UNP Q12109
C	438	HIS	-	EXPRESSION TAG	UNP Q12109
D	433	HIS	-	EXPRESSION TAG	UNP Q12109
D	434	HIS	-	EXPRESSION TAG	UNP Q12109
D	435	HIS	-	EXPRESSION TAG	UNP Q12109

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Chain	Residue	Modelled	Actual	Comment	Reference
D	436	HIS	-	EXPRESSION TAG	UNP Q12109
D	437	HIS	-	EXPRESSION TAG	UNP Q12109
D	438	HIS	-	EXPRESSION TAG	UNP Q12109

- Molecule 2 is L-TRYPTOPHANAMIDE (three-letter code: LTN) (formula: $C_{11}H_{13}N_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	11	3	1		
2	B	1	Total	C	N	O	0	0
			15	11	3	1		
2	C	1	Total	C	N	O	0	0
			15	11	3	1		
2	D	1	Total	C	N	O	0	0
			15	11	3	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total 1	O 1	0	0
4	D	8	Total 8	O 8	0	0

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.

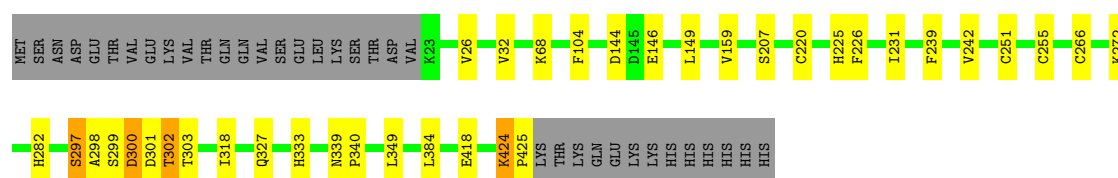
- Molecule 1: Tryptophanyl-tRNA synthetase, cytoplasmic

Chain A:



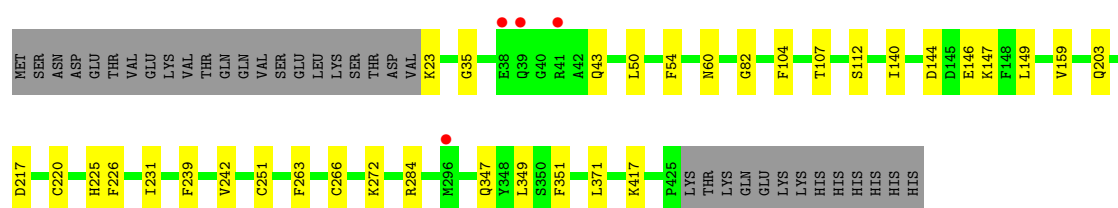
- Molecule 1: Tryptophanyl-tRNA synthetase, cytoplasmic

Chain B:



- Molecule 1: Tryptophanyl-tRNA synthetase, cytoplasmic

Chain C:



- Molecule 1: Tryptophanyl-tRNA synthetase, cytoplasmic

Chain D:



F239	P240	N241	V242	L243	G244	I253	D260	P261	C266	L280	A288	L289	Q290	G291	T294	D300	D301	T302	T303	T310	Q313	Q327	H333	S350	L359	K360	L371	K411	P425	LYS	THR	LYS	GLN	LYS	LYS	HIS	HIS	HIS	HIS	HIS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	252.26Å 252.26Å 111.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.04 – 3.00 49.04 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.8 (49.04-3.00) 97.7 (49.04-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.247 , 0.273 0.243 , 0.241	Depositor DCC
R_{free} test set	3960 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	71.9	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.5	EDS
Estimated twinning fraction	0.008 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 79189 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13222	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, LTN

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	0.33	0/3369	0.45	0/4546
1	B	0.33	0/3332	0.47	1/4496 (0.0%)
1	C	0.33	0/3332	0.44	0/4496
1	D	0.33	0/3386	0.46	0/4569
All	All	0.33	0/13419	0.46	1/18107 (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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	298	ALA	N-CA-C	-8.72	87.45	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	297	SER	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3287	0	3247	26	0
1	B	3250	0	3209	19	0
1	C	3250	0	3209	15	0
1	D	3304	0	3264	22	0
2	A	15	0	13	0	0
2	B	15	0	13	0	0
2	C	15	0	13	0	0
2	D	15	0	13	0	0
3	A	15	0	0	0	0
3	B	15	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
4	A	6	0	0	0	0
4	B	6	0	0	0	0
4	C	1	0	0	0	0
4	D	8	0	0	0	0
All	All	13222	0	12981	77	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

The worst 5 of 77 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:310:THR:H	1:A:313:GLN:HE21	1.28	0.79
1:D:28:THR:HG22	1:D:29:PRO:HD2	1.71	0.72
1:A:179:ASN:H	1:A:179:ASN:HD22	1.45	0.64
1:C:239:PHE:HB3	1:C:242:VAL:HB	1.81	0.63
1:D:288:ALA:HB3	1:D:294:THR:HG23	1.82	0.62

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	406/438 (93%)	396 (98%)	10 (2%)	0	100	100
1	B	401/438 (92%)	387 (96%)	13 (3%)	1 (0%)	56	92
1	C	401/438 (92%)	387 (96%)	14 (4%)	0	100	100
1	D	408/438 (93%)	396 (97%)	11 (3%)	1 (0%)	56	92
All	All	1616/1752 (92%)	1566 (97%)	48 (3%)	2 (0%)	59	93

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	301	ASP
1	D	29	PRO

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	361/391 (92%)	349 (97%)	12 (3%)	50	88
1	B	356/391 (91%)	349 (98%)	7 (2%)	68	94
1	C	356/391 (91%)	349 (98%)	7 (2%)	68	94
1	D	363/391 (93%)	347 (96%)	16 (4%)	39	82
All	All	1436/1564 (92%)	1394 (97%)	42 (3%)	55	90

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	424	LYS
1	C	349	LEU

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Mol	Chain	Res	Type
1	D	290	GLN
1	C	23	LYS
1	C	149	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	333	HIS
1	C	60	ASN
1	D	241	ASN
1	B	290	GLN
1	D	313	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

14 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	439	-	4,4,4	0.22	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	440	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	A	441	-	4,4,4	0.21	0	6,6,6	0.08	0
2	LTN	A	500	-	16,16,16	1.18	1 (6%)	22,22,22	0.60	0
3	SO4	B	439	-	4,4,4	0.21	0	6,6,6	0.07	0
3	SO4	B	440	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	B	441	-	4,4,4	0.10	0	6,6,6	0.14	0
2	LTN	B	700	-	16,16,16	1.19	2 (12%)	22,22,22	0.62	0
3	SO4	C	439	-	4,4,4	0.23	0	6,6,6	0.11	0
3	SO4	C	440	-	4,4,4	0.23	0	6,6,6	0.06	0
2	LTN	C	600	-	16,16,16	1.17	1 (6%)	22,22,22	0.61	0
3	SO4	D	439	-	4,4,4	0.21	0	6,6,6	0.08	0
3	SO4	D	440	-	4,4,4	0.22	0	6,6,6	0.08	0
2	LTN	D	800	-	16,16,16	1.19	1 (6%)	22,22,22	0.61	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	439	-	-	0/0/0/0	0/0/0/0
3	SO4	A	440	-	-	0/0/0/0	0/0/0/0
3	SO4	A	441	-	-	0/0/0/0	0/0/0/0
2	LTN	A	500	-	-	0/8/8/8	0/0/2/2
3	SO4	B	439	-	-	0/0/0/0	0/0/0/0
3	SO4	B	440	-	-	0/0/0/0	0/0/0/0
3	SO4	B	441	-	-	0/0/0/0	0/0/0/0
2	LTN	B	700	-	-	0/8/8/8	0/0/2/2
3	SO4	C	439	-	-	0/0/0/0	0/0/0/0
3	SO4	C	440	-	-	0/0/0/0	0/0/0/0
2	LTN	C	600	-	-	0/8/8/8	0/0/2/2
3	SO4	D	439	-	-	0/0/0/0	0/0/0/0
3	SO4	D	440	-	-	0/0/0/0	0/0/0/0
2	LTN	D	800	-	-	0/8/8/8	0/0/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	800	LTN	CD1-CG	-2.70	1.33	1.37
2	B	700	LTN	CD1-CG	-2.65	1.33	1.37
2	A	500	LTN	CD1-CG	-2.62	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	600	LTN	CD1-CG	-2.58	1.33	1.37
2	B	700	LTN	CD1-NE1	-2.01	1.33	1.37

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th 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 ²)	Q<0.9
1	A	408/438 (93%)	-0.10	0	100	100	63, 72, 96, 106	0
1	B	403/438 (92%)	0.00	0	100	100	49, 83, 120, 135	0
1	C	403/438 (92%)	-0.00	4 (0%)	79	22	61, 74, 112, 122	0
1	D	410/438 (93%)	-0.07	0	100	100	70, 83, 100, 109	0
All	All	1624/1752 (92%)	-0.04	4 (0%)	93	54	49, 78, 106, 135	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	296	MET	2.6
1	C	41	ARG	2.5
1	C	39	GLN	2.3
1	C	38	GLU	2.2

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	SO4	C	439	5/5	0.23	1.95	64,64,64,64	5
2	LTN	C	600	15/15	0.26	0.37	74,74,75,75	0
3	SO4	D	439	5/5	0.20	0.35	80,80,80,80	5
3	SO4	A	441	5/5	0.24	0.05	78,78,78,78	5
3	SO4	C	440	5/5	0.34	-0.08	100,100,100,100	5
3	SO4	B	441	5/5	0.25	-0.36	102,102,102,102	5
3	SO4	B	439	5/5	0.17	-0.49	89,89,89,89	5
2	LTN	B	700	15/15	0.21	-0.58	78,79,79,79	0
2	LTN	D	800	15/15	0.19	-0.95	73,73,73,73	0
3	SO4	B	440	5/5	0.17	-1.19	82,82,82,82	5
2	LTN	A	500	15/15	0.18	-1.70	68,68,68,68	0
3	SO4	A	440	5/5	0.18	-1.83	81,81,81,81	5
3	SO4	D	440	5/5	0.14	-2.50	59,59,59,59	5
3	SO4	A	439	5/5	0.12	-9.88	102,102,102,102	5

6.5 Other polymers ⓘ

There are no such residues in this entry.