WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 09:38 AM GMT

PDB ID : 3KT6

Title : Crystal structure of S. cerevisiae tryptophanyl-tRNA synthetase in complex with Trp

Authors : Zhou, M.; Dong, X.; Zhong, C.; Shen, N.; Ding, J.

Deposited on : 2009-11-24

Resolution : 2.80 Å(reported)

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 2.80 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	Percentile Ranks	Value
Rfree		0.214
Clashscore		1
Ramachandran outliers		0
Sidechain outliers		3.9%
RSRZ outliers		2.6%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
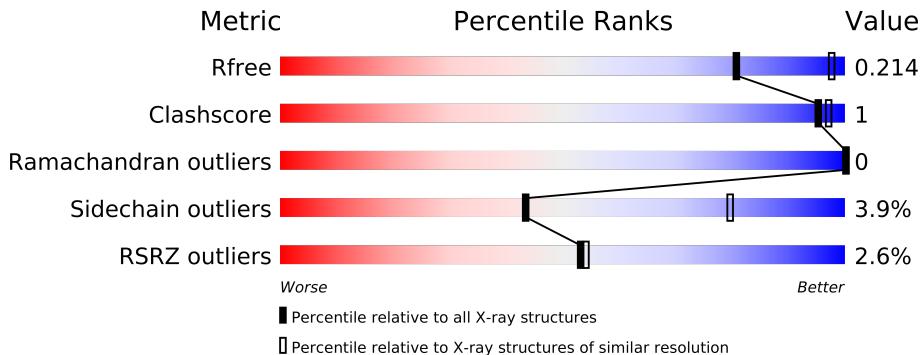
| Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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	
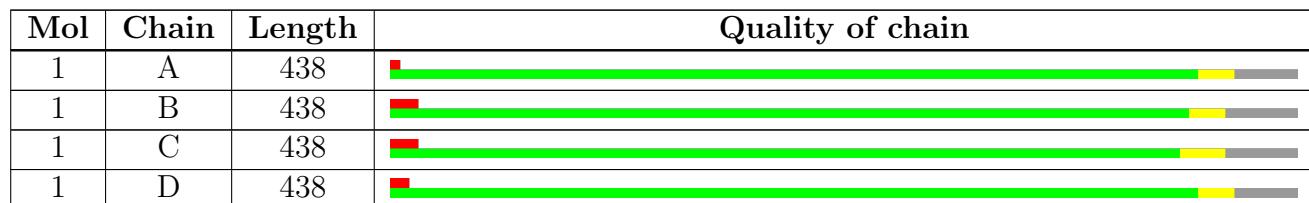
2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 13292 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	409	Total	C	N	O	S	0	0	0
			3295	2124	546	612	13			
1	B	404	Total	C	N	O	S	0	0	0
			3257	2101	540	603	13			
1	C	404	Total	C	N	O	S	0	0	0
			3257	2101	540	603	13			
1	D	409	Total	C	N	O	S	0	0	0
			3295	2124	546	612	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 TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).
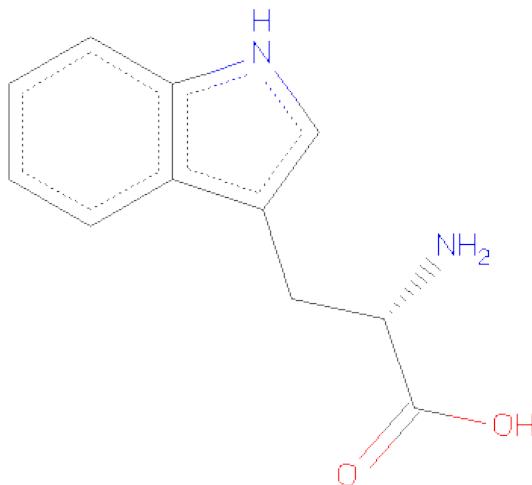
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 15	C 11	N 2	O 2	0	0
2	B	1	Total 15	C 11	N 2	O 2	0	0
2	C	1	Total 15	C 11	N 2	O 2	0	0
2	D	1	Total 15	C 11	N 2	O 2	0	0

• Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
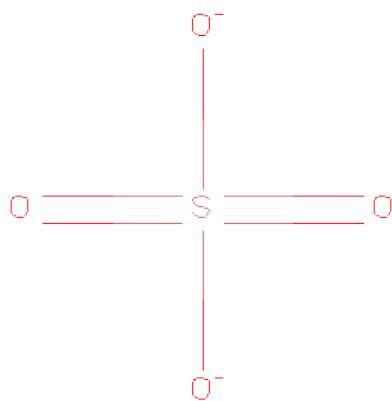
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	C	1	Total 5	O 4	S 1	0	0
3	C	1	Total 5	O 4	S 1	0	0
3	C	1	Total 5	O 4	S 1	0	0
3	D	1	Total 5	O 4	S 1	0	0
3	D	1	Total 5	O 4	S 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	25	Total 25	O 25	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	20	Total 20	O 20	0	0
4	C	17	Total 17	O 17	0	0
4	D	11	Total 11	O 11	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.
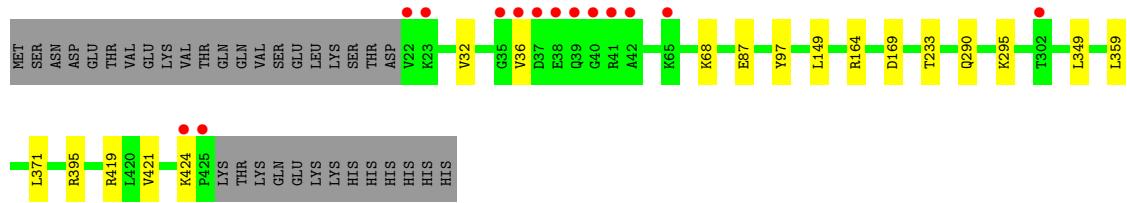
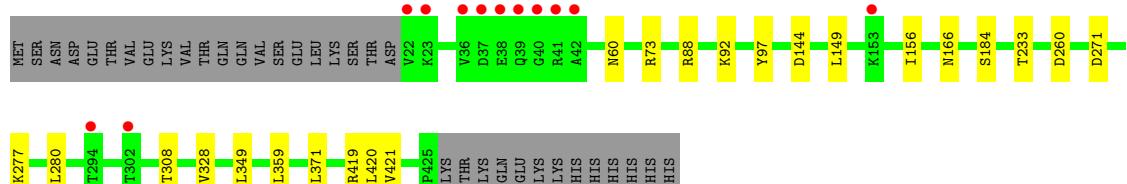- Molecule 1: Tryptophanyl-tRNA synthetase, cytoplasmic

Chain A:
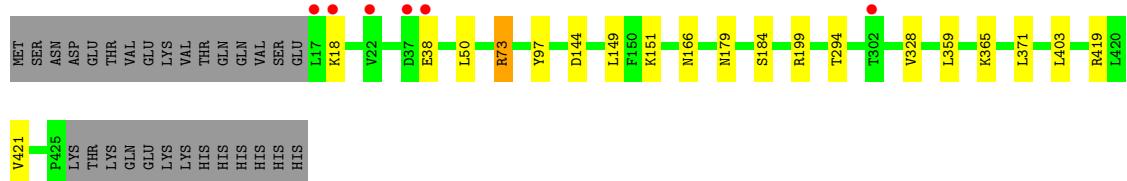
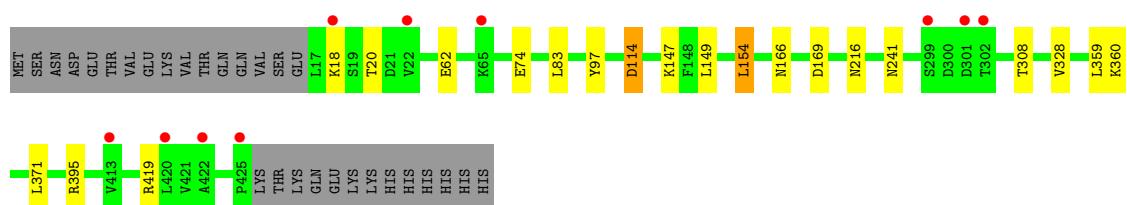- Molecule 1: Tryptophanyl-tRNA synthetase, cytoplasmic

Chain B:

- Molecule 1: Tryptophanyl-tRNA synthetase, cytoplasmic

Chain C:

- Molecule 1: Tryptophanyl-tRNA synthetase, cytoplasmic

Chain D:

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	252.66Å 252.66Å 111.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.75 – 2.80 47.75 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.75-2.80) 99.4 (47.75-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.35 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.216 , 0.247 0.213 , 0.214	Depositor DCC
R_{free} test set	4964 reflections (5.25%)	DCC
Wilson B-factor (Å^2)	61.5	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 31.8	EDS
Estimated twinning fraction	0.012 for h,-h-k,-l	Xtriage
L-test for twinning	$< |L| > = 0.52, < L^2 > = 0.36$	Xtriage
Outliers	0 of 99521 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13292	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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	A	0.42	1/3377 (0.0%)	0.49	0/4557
1	B	0.37	0/3339	0.48	0/4506
1	C	0.38	0/3339	0.49	0/4506
1	D	0.38	0/3377	0.49	1/4557 (0.0%)
All	All	0.39	1/13432 (0.0%)	0.49	1/18126 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	GLU	CD-OE1	8.90	1.35	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	154	LEU	CA-CB-CG	5.35	127.60	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 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	3295	0	0	4	0
1	B	3257	0	0	2	0
1	C	3257	0	0	6	0
1	D	3295	0	0	5	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0
2	C	15	0	0	0	0
2	D	15	0	0	0	0
3	A	20	0	0	2	0
3	B	10	0	0	0	0
3	C	15	0	0	2	0
3	D	10	0	0	0	0
4	A	25	0	0	0	0
4	B	20	0	0	0	0
4	C	17	0	0	0	0
4	D	11	0	0	1	0
All	All	13292	0	0	17	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 1.

All (17) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:97:TYR:O	1:A:419:ARG:NH2	2.27	0.67
1:C:97:TYR:O	1:C:419:ARG:NH2	2.33	0.61
1:C:88:ARG:NH2	1:C:260:ASP:OD1	2.34	0.60
1:B:97:TYR:O	1:B:419:ARG:NH2	2.35	0.58
1:A:199:ARG:NE	3:A:503:SO4:O2	2.38	0.56
1:C:73:ARG:NE	3:C:602:SO4:O1	2.39	0.53
1:C:156:ILE:N	3:C:603:SO4:O4	2.46	0.49
1:C:144:ASP:OD2	1:C:184:SER:OG	2.31	0.48
1:D:97:TYR:O	1:D:419:ARG:NH2	2.49	0.45
1:D:169:ASP:OD1	1:D:395:ARG:NE	2.49	0.45
1:D:241:ASN:ND2	4:D:808:HOH:O	2.50	0.44
1:C:92:LYS:NZ	1:C:277:LYS:O	2.50	0.44
1:D:114:ASP:OD1	1:D:114:ASP:N	2.51	0.43
1:A:73:ARG:CD	3:A:502:SO4:O3	2.68	0.42
1:D:74:GLU:N	1:D:74:GLU:OE1	2.54	0.41
1:A:144:ASP:OD2	1:A:184:SER:OG	2.39	0.40
1:B:169:ASP:OD1	1:B:395:ARG:NE	2.55	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	407/438 (93%)	397 (98%)	10 (2%)	0	100	100
1	B	402/438 (92%)	389 (97%)	13 (3%)	0	100	100
1	C	402/438 (92%)	391 (97%)	11 (3%)	0	100	100
1	D	407/438 (93%)	395 (97%)	12 (3%)	0	100	100
All	All	1618/1752 (92%)	1572 (97%)	46 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	362/391 (93%)	348 (96%)	14 (4%)	43	80
1	B	357/391 (91%)	343 (96%)	14 (4%)	43	80
1	C	357/391 (91%)	344 (96%)	13 (4%)	47	82
1	D	362/391 (93%)	347 (96%)	15 (4%)	41	77
All	All	1438/1564 (92%)	1382 (96%)	56 (4%)	43	80

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	50	LEU
1	A	73	ARG
1	A	149	LEU
1	A	151	LYS

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Mol	Chain	Res	Type
1	A	166	ASN
1	A	179	ASN
1	A	294	THR
1	A	328	VAL
1	A	359	LEU
1	A	365	LYS
1	A	371	LEU
1	A	403	LEU
1	A	421	VAL
1	B	32	VAL
1	B	36	VAL
1	B	68	LYS
1	B	87	GLU
1	B	149	LEU
1	B	164	ARG
1	B	233	THR
1	B	290	GLN
1	B	295	LYS
1	B	349	LEU
1	B	359	LEU
1	B	371	LEU
1	B	421	VAL
1	B	424	LYS
1	C	60	ASN
1	C	149	LEU
1	C	166	ASN
1	C	233	THR
1	C	271	ASP
1	C	280	LEU
1	C	308	THR
1	C	328	VAL
1	C	349	LEU
1	C	359	LEU
1	C	371	LEU
1	C	420	LEU
1	C	421	VAL
1	D	18	LYS
1	D	20	THR
1	D	62	GLU
1	D	83	LEU
1	D	114	ASP
1	D	147	LYS

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Mol	Chain	Res	Type
1	D	149	LEU
1	D	154	LEU
1	D	166	ASN
1	D	216	ASN
1	D	308	THR
1	D	328	VAL
1	D	359	LEU
1	D	360	LYS
1	D	371	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3   RNA   (i)

There are no RNA chains in this entry.

5.4   Non-standard residues in protein, DNA, RNA chains   (i)

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

5.5   Carbohydrates   (i)

There are no carbohydrates in this entry.

5.6   Ligand geometry   (i)

15 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	$\#|Z| > 2$
2	TRP	A	500	-	16,16,16	0.74	0	22,22,22	1.06	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	SO4	A	501	-	4,4,4	0.16	0	6,6,6	0.11	0
3	SO4	A	502	-	4,4,4	0.28	0	6,6,6	0.14	0
3	SO4	A	503	-	4,4,4	0.12	0	6,6,6	0.20	0
3	SO4	A	703	-	4,4,4	0.22	0	6,6,6	0.24	0
2	TRP	B	700	-	16,16,16	0.76	0	22,22,22	1.00	1 (4%)
3	SO4	B	701	-	4,4,4	0.20	0	6,6,6	0.09	0
3	SO4	B	702	-	4,4,4	0.07	0	6,6,6	0.08	0
2	TRP	C	600	-	16,16,16	0.84	0	22,22,22	1.03	1 (4%)
3	SO4	C	601	-	4,4,4	0.17	0	6,6,6	0.12	0
3	SO4	C	602	-	4,4,4	0.21	0	6,6,6	0.16	0
3	SO4	C	603	-	4,4,4	0.16	0	6,6,6	0.22	0
2	TRP	D	800	-	16,16,16	0.75	0	22,22,22	0.96	1 (4%)
3	SO4	D	801	-	4,4,4	0.34	0	6,6,6	0.11	0
3	SO4	D	802	-	4,4,4	0.14	0	6,6,6	0.22	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
2	TRP	A	500	-	-	0/8/8/8	0/0/2/2
3	SO4	A	501	-	-	0/0/0/0	0/0/0/0
3	SO4	A	502	-	-	0/0/0/0	0/0/0/0
3	SO4	A	503	-	-	0/0/0/0	0/0/0/0
3	SO4	A	703	-	-	0/0/0/0	0/0/0/0
2	TRP	B	700	-	-	0/8/8/8	0/0/2/2
3	SO4	B	701	-	-	0/0/0/0	0/0/0/0
3	SO4	B	702	-	-	0/0/0/0	0/0/0/0
2	TRP	C	600	-	-	0/8/8/8	0/0/2/2
3	SO4	C	601	-	-	0/0/0/0	0/0/0/0
3	SO4	C	602	-	-	0/0/0/0	0/0/0/0
3	SO4	C	603	-	-	0/0/0/0	0/0/0/0
2	TRP	D	800	-	-	0/8/8/8	0/0/2/2
3	SO4	D	801	-	-	0/0/0/0	0/0/0/0
3	SO4	D	802	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	TRP	OXT-C-O	-2.94	117.43	124.07
2	C	600	TRP	OXT-C-O	-2.68	118.00	124.07
2	B	700	TRP	OXT-C-O	-2.67	118.03	124.07
2	D	800	TRP	OXT-C-O	-2.57	118.26	124.07

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(Å²)	Q<0.9
1	A	409/438 (93%)	-0.22	6 (1%)	70	71	42, 58, 98, 141	0
1	B	404/438 (92%)	-0.01	14 (3%)	42	42	35, 64, 104, 156	0
1	C	404/438 (92%)	-0.12	12 (2%)	48	49	36, 59, 110, 151	0
1	D	409/438 (93%)	0.01	10 (2%)	56	57	49, 71, 107, 138	0
All	All	1626/1752 (92%)	-0.09	42 (2%)	53	54	35, 63, 105, 156	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	39	GLN	4.1
1	C	41	ARG	4.0
1	B	22	VAL	4.0
1	C	22	VAL	3.9
1	A	22	VAL	3.8
1	C	38	GLU	3.7
1	B	40	GLY	3.7
1	C	23	LYS	3.6
1	B	302	THR	3.4
1	B	39	GLN	3.4
1	B	37	ASP	3.4
1	A	18	LYS	3.3
1	D	18	LYS	3.1
1	B	38	GLU	3.1
1	C	40	GLY	3.0
1	C	36	VAL	3.0
1	B	23	LYS	3.0
1	B	41	ARG	2.9
1	D	420	LEU	2.8
1	B	36	VAL	2.7
1	C	294	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	35	GLY	2.6
1	D	422	ALA	2.6
1	D	22	VAL	2.5
1	A	302	THR	2.5
1	D	299	SER	2.5
1	C	302	THR	2.4
1	A	37	ASP	2.4
1	B	42	ALA	2.4
1	C	37	ASP	2.3
1	B	424	LYS	2.3
1	D	413	VAL	2.3
1	D	65	LYS	2.2
1	D	425	PRO	2.2
1	C	42	ALA	2.2
1	B	425	PRO	2.2
1	B	65	LYS	2.2
1	D	301	ASP	2.1
1	A	17	LEU	2.1
1	A	38	GLU	2.1
1	C	153	LYS	2.1
1	D	302	THR	2.0

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(Å^2)	Q<0.9
2	TRP	B	700	15/15	0.24	1.83	53,54,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	TRP	A	500	15/15	0.22	1.83	56,56,62,62	0
3	SO4	B	701	5/5	0.24	1.72	83,87,87,87	0
2	TRP	D	800	15/15	0.22	1.58	72,72,74,74	0
2	TRP	C	600	15/15	0.22	0.65	49,50,53,53	0
3	SO4	C	603	5/5	0.20	0.47	45,56,57,57	5
3	SO4	D	801	5/5	0.19	0.01	90,95,95,95	5
3	SO4	A	503	5/5	0.16	-0.22	43,56,57,57	5
3	SO4	A	501	5/5	0.17	-0.34	89,95,95,95	5
3	SO4	A	703	5/5	0.16	-0.45	42,54,56,56	5
3	SO4	D	802	5/5	0.16	-0.51	41,53,55,55	5
3	SO4	B	702	5/5	0.16	-0.51	44,56,57,57	5
3	SO4	C	601	5/5	0.15	-1.02	48,60,62,62	5
3	SO4	C	602	5/5	0.12	-5.71	38,52,53,53	5
3	SO4	A	502	5/5	0.14	-10.14	45,58,59,60	5

6.5 Other polymers ⓘ

There are no such residues in this entry.