



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2020 – 01:03 pm BST

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)

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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

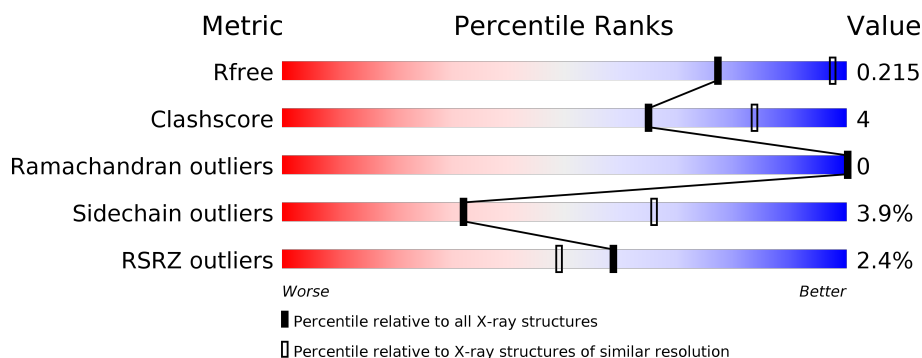
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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  $\geq 3$ , 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	438	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>13%</div> <div>7%</div> </div> </div>
1	B	438	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>8%</div> </div> </div>
1	C	438	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>12%</div> <div>8%</div> </div> </div>
1	D	438	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>7%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	502	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13292 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 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:

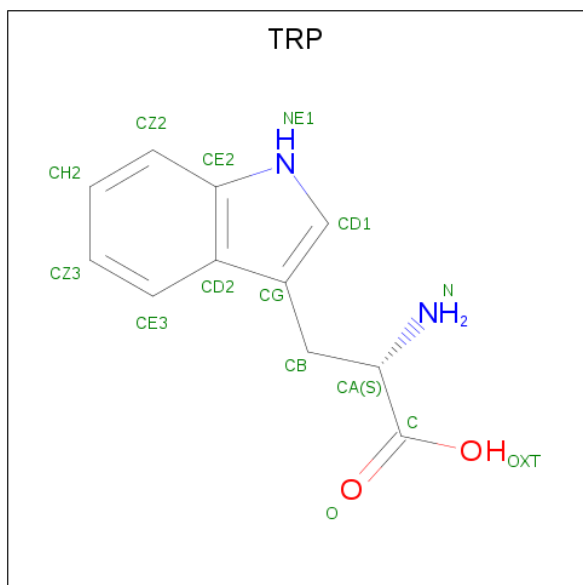
Chain	Residue	Modelled	Actual	Comment	Reference
A	433	HIS	-	EXPRESSION TAG	UNP Q12109
A	434	HIS	-	EXPRESSION TAG	UNP Q12109
A	435	HIS	-	EXPRESSION TAG	UNP Q12109
A	436	HIS	-	EXPRESSION TAG	UNP Q12109
A	437	HIS	-	EXPRESSION TAG	UNP Q12109
A	438	HIS	-	EXPRESSION TAG	UNP Q12109
B	433	HIS	-	EXPRESSION TAG	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	C	N	O	0	0
			15	11	2	2		
2	B	1	Total	C	N	O	0	0
			15	11	2	2		
2	C	1	Total	C	N	O	0	0
			15	11	2	2		
2	D	1	Total	C	N	O	0	0
			15	11	2	2		

- 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	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	C	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	25	Total	O	0	0
			25	25		

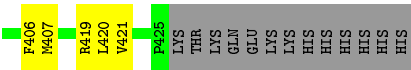
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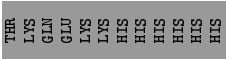
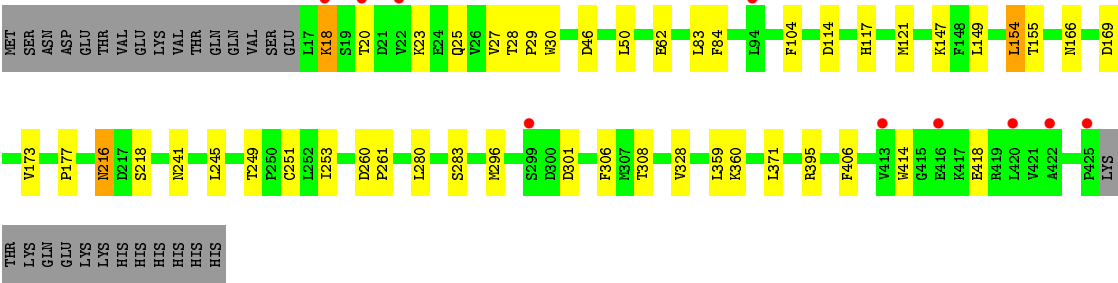
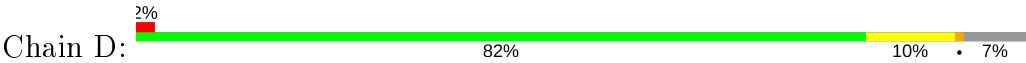
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	20	Total	O	0	0
			20	20		
4	C	17	Total	O	0	0
			17	17		
4	D	11	Total	O	0	0
			11	11		







● Molecule 1: Tryptophanyl-tRNA synthetase, cytoplasmic



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.35 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.216 , 0.247 0.213 , 0.215	Depositor DCC
$R_{free}$ test set	4964 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.5	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.012 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13292	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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	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(°)	Ideal(°)
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 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	3295	0	3258	36	0
1	B	3257	0	3218	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3257	0	3218	27	0
1	D	3295	0	3258	24	0
2	A	15	0	9	0	0
2	B	15	0	9	0	0
2	C	15	0	9	0	0
2	D	15	0	9	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	1	0
4	A	25	0	0	1	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	12988	107	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 4.

All (107) 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:310:THR:H	1:A:313:GLN:HE21	1.33	0.75
1:C:310:THR:H	1:C:313:GLN:HE21	1.41	0.67
1:A:179:ASN:H	1:A:179:ASN:HD22	1.43	0.65
1:A:310:THR:H	1:A:313:GLN:NE2	1.95	0.64
1:A:330:ALA:O	1:A:334:ARG:HG2	1.99	0.62
1:B:318:ILE:HD11	1:B:384:LEU:HD12	1.82	0.62
1:A:418:GLU:H	1:A:418:GLU:CD	2.01	0.62
1:C:88:ARG:NH2	1:C:260:ASP:OD1	2.34	0.59
1:C:23:LYS:HB3	1:C:36:VAL:HG22	1.85	0.59
1:B:285:PHE:HB3	1:B:295:LYS:HB3	1.86	0.58
1:A:77:HIS:HB2	1:A:81:LYS:HE3	1.87	0.57
1:A:253:ILE:HB	1:A:280:LEU:HD23	1.86	0.56
1:A:26:VAL:HG21	1:D:23:LYS:HD3	1.86	0.56
1:A:146:GLU:HB2	1:A:226:PHE:CZ	2.41	0.56
1:C:239:PHE:HB3	1:C:242:VAL:HB	1.87	0.55
1:D:18:LYS:H	1:D:18:LYS:HD3	1.71	0.54
1:C:310:THR:H	1:C:313:GLN:NE2	2.05	0.53
1:B:116:MET:CE	1:B:169:ASP:HB2	2.39	0.53
1:B:97:TYR:O	1:B:419:ARG:NH2	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:HIS:CE1	1:D:296:MET:HG2	2.45	0.51
1:A:66:ARG:HG2	1:A:94:LEU:HD13	1.92	0.51
1:C:32:VAL:HG11	1:C:295:LYS:HD3	1.91	0.51
1:D:253:ILE:HB	1:D:280:LEU:HD23	1.91	0.51
1:A:67:PHE:HZ	1:A:133:VAL:HG11	1.76	0.51
1:C:67:PHE:HZ	1:C:133:VAL:HG11	1.75	0.51
1:C:104:PHE:CZ	1:C:251:CYS:HB3	2.46	0.51
1:A:110:GLY:HA3	1:A:147:LYS:HE3	1.91	0.50
1:A:239:PHE:HB3	1:A:242:VAL:HB	1.92	0.50
1:A:112:SER:HB3	1:A:147:LYS:HD2	1.93	0.49
1:C:60:ASN:HD22	1:C:60:ASN:C	2.14	0.49
1:D:25:GLN:HE22	1:D:46:ASP:H	1.59	0.49
1:A:87:GLU:HB3	1:A:281:LEU:HD23	1.94	0.49
1:D:260:ASP:N	1:D:261:PRO:HD2	2.26	0.49
1:A:334:ARG:HG3	4:A:521:HOH:O	2.12	0.49
1:C:245:LEU:HD13	1:C:249:THR:HG21	1.94	0.49
1:C:67:PHE:CZ	1:C:133:VAL:HG11	2.48	0.48
1:A:104:PHE:CZ	1:A:251:CYS:HB3	2.49	0.48
1:C:36:VAL:HG12	1:C:42:ALA:HA	1.94	0.48
1:D:301:ASP:HA	1:D:306:PHE:HE2	1.79	0.47
1:B:239:PHE:HB3	1:B:242:VAL:HB	1.97	0.47
1:B:32:VAL:HG11	1:B:295:LYS:HG2	1.97	0.47
1:A:121:MET:HE1	1:A:173:VAL:HG22	1.97	0.47
1:C:155:THR:HG22	1:C:157:ASN:H	1.78	0.47
1:B:107:THR:O	1:B:140:ILE:HA	2.15	0.47
1:D:104:PHE:CZ	1:D:251:CYS:HB3	2.50	0.47
1:D:84:PHE:CE2	1:D:283:SER:HB3	2.50	0.46
1:B:137:PRO:HD3	1:B:414:TRP:CG	2.50	0.46
1:D:418:GLU:H	1:D:418:GLU:CD	2.19	0.46
1:B:146:GLU:HB2	1:B:226:PHE:CZ	2.51	0.46
1:D:245:LEU:HD21	1:D:414:TRP:HZ2	1.81	0.46
1:C:84:PHE:CZ	1:C:283:SER:HB3	2.51	0.46
1:D:84:PHE:CZ	1:D:283:SER:HB3	2.51	0.46
1:B:77:HIS:HB2	1:B:81:LYS:HE3	1.97	0.46
1:A:118:LEU:HD21	1:A:384:LEU:HD22	1.97	0.45
1:A:135:ASP:OD2	1:A:417:LYS:HG2	2.16	0.45
1:D:28:THR:HG22	1:D:30:TRP:H	1.82	0.45
1:B:116:MET:HE2	1:B:169:ASP:HB2	1.99	0.45
1:C:146:GLU:HB2	1:C:226:PHE:CZ	2.52	0.44
1:C:263:PHE:HA	1:C:266:CYS:HB3	1.99	0.44
1:B:144:ASP:HB2	1:B:159:VAL:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LEU:HD13	1:A:249:THR:HG21	1.99	0.44
1:C:73:ARG:NE	3:C:602:SO4:O1	2.39	0.44
1:C:176:ASP:OD1	1:C:177:PRO:HD2	2.17	0.44
1:D:245:LEU:HD13	1:D:249:THR:HG21	2.00	0.44
1:B:84:PHE:CZ	1:B:283:SER:HB3	2.53	0.44
1:D:121:MET:CE	1:D:173:VAL:HG22	2.48	0.44
1:B:104:PHE:CZ	1:B:251:CYS:HB3	2.53	0.44
1:C:182:ILE:O	1:C:407:MET:HA	2.18	0.43
1:D:216:ASN:C	1:D:216:ASN:HD22	2.21	0.43
1:A:179:ASN:N	1:A:179:ASN:HD22	2.07	0.43
1:A:225:HIS:HB2	1:B:225:HIS:HB2	2.00	0.43
1:C:177:PRO:HD3	1:C:406:PHE:CZ	2.53	0.43
1:D:121:MET:HE1	1:D:173:VAL:HG22	2.00	0.43
1:C:74:GLU:HG2	1:C:75:PRO:HD2	2.00	0.43
1:A:182:ILE:O	1:A:407:MET:HA	2.18	0.43
1:A:73:ARG:HH21	1:A:73:ARG:CG	2.31	0.43
1:D:27:VAL:HG21	1:D:50:LEU:HD11	2.01	0.43
1:A:67:PHE:CZ	1:A:133:VAL:HG11	2.53	0.43
1:A:365:LYS:HB3	1:A:371:LEU:HB2	2.01	0.43
1:C:144:ASP:HB2	1:C:159:VAL:HB	2.01	0.43
1:B:231:ILE:HG12	1:B:266:CYS:HB2	2.00	0.42
1:C:97:TYR:O	1:C:419:ARG:NH2	2.33	0.42
1:C:155:THR:HG23	3:C:603:SO4:O4	2.19	0.42
1:D:169:ASP:OD1	1:D:395:ARG:NE	2.49	0.42
1:B:193:PHE:CE1	1:B:233:THR:HG22	2.55	0.42
1:B:289:LEU:O	1:B:322:ALA:HA	2.20	0.42
1:D:241:ASN:ND2	4:D:808:HOH:O	2.50	0.42
1:A:73:ARG:CD	3:A:502:SO4:O3	2.68	0.42
1:B:229:ILE:O	1:B:233:THR:HG23	2.20	0.42
1:A:121:MET:CE	1:A:173:VAL:HG22	2.50	0.41
1:D:216:ASN:HD22	1:D:218:SER:H	1.68	0.41
1:D:155:THR:HB	3:D:802:SO4:O3	2.20	0.41
1:A:231:ILE:HG12	1:A:266:CYS:HB2	2.03	0.41
1:A:97:TYR:O	1:A:419:ARG:NH2	2.27	0.41
1:A:229:ILE:O	1:A:233:THR:HG23	2.21	0.41
1:B:26:VAL:O	1:B:32:VAL:HA	2.20	0.41
1:D:28:THR:HG23	1:D:29:PRO:HD2	2.03	0.41
1:C:104:PHE:CE2	1:C:251:CYS:HB3	2.55	0.41
1:A:289:LEU:HD21	1:A:317:LYS:HB3	2.03	0.41
1:A:147:LYS:HA	1:A:147:LYS:HD3	1.79	0.41
1:B:263:PHE:HA	1:B:266:CYS:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:THR:O	1:C:140:ILE:HA	2.21	0.40
1:A:18:LYS:CE	1:A:19:SER:H	2.35	0.40
1:D:177:PRO:HD3	1:D:406:PHE:CZ	2.57	0.40
1:C:306:PHE:C	1:C:308:THR:H	2.24	0.40
1:A:73:ARG:HD2	3:A:502:SO4:O3	2.21	0.40
1:B:116:MET:HE3	1:B:169:ASP:HB2	2.01	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	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 [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	
1	A	362/391 (93%)	348 (96%)	14 (4%)	32	66
1	B	357/391 (91%)	343 (96%)	14 (4%)	32	66
1	C	357/391 (91%)	344 (96%)	13 (4%)	35	69
1	D	362/391 (93%)	347 (96%)	15 (4%)	30	64
All	All	1438/1564 (92%)	1382 (96%)	56 (4%)	32	66

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
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

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Mol	Chain	Res	Type
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
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. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	179	ASN
1	A	313	GLN
1	A	385	GLN
1	B	43	GLN
1	B	385	GLN
1	C	60	ASN
1	C	131	GLN
1	C	290	GLN
1	C	313	GLN
1	C	385	GLN
1	D	25	GLN
1	D	53	GLN
1	D	216	ASN
1	D	313	GLN

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Mol	Chain	Res	Type
1	D	385	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules 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	$\# Z  > 2$
3	SO4	A	501	-	4,4,4	0.14	0	6,6,6	0.09	0
3	SO4	C	603	-	4,4,4	0.17	0	6,6,6	0.20	0
3	SO4	B	702	-	4,4,4	0.17	0	6,6,6	0.07	0
3	SO4	C	601	-	4,4,4	0.17	0	6,6,6	0.17	0
3	SO4	A	503	-	4,4,4	0.14	0	6,6,6	0.21	0
3	SO4	A	703	-	4,4,4	0.26	0	6,6,6	0.21	0
3	SO4	D	802	-	4,4,4	0.21	0	6,6,6	0.21	0
3	SO4	C	602	-	4,4,4	0.15	0	6,6,6	0.17	0
3	SO4	D	801	-	4,4,4	0.23	0	6,6,6	0.12	0
3	SO4	A	502	-	4,4,4	0.31	0	6,6,6	0.12	0
3	SO4	B	701	-	4,4,4	0.16	0	6,6,6	0.11	0

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.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	603	SO4	1	0
3	D	802	SO4	1	0
3	C	602	SO4	1	0
3	A	502	SO4	2	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	409/438 (93%)	-0.15	7 (1%) 70 63	42, 58, 98, 141	0
1	B	404/438 (92%)	-0.03	11 (2%) 54 44	35, 64, 104, 156	0
1	C	404/438 (92%)	-0.02	11 (2%) 54 44	36, 59, 110, 151	0
1	D	409/438 (93%)	0.00	10 (2%) 59 49	49, 71, 107, 138	0
All	All	1626/1752 (92%)	-0.05	39 (2%) 59 49	35, 63, 105, 156	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	22	VAL	4.2
1	A	22	VAL	4.1
1	C	23	LYS	3.6
1	C	41	ARG	3.6
1	C	38	GLU	3.4
1	D	420	LEU	3.3
1	C	36	VAL	3.3
1	B	22	VAL	3.2
1	C	39	GLN	3.1
1	A	21	ASP	3.0
1	B	40	GLY	2.8
1	B	37	ASP	2.8
1	D	18	LYS	2.8
1	B	23	LYS	2.7
1	B	302	THR	2.7
1	B	39	GLN	2.7
1	B	38	GLU	2.7
1	A	37	ASP	2.6
1	D	22	VAL	2.5
1	C	40	GLY	2.5
1	D	299	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	294	THR	2.4
1	A	302	THR	2.4
1	D	413	VAL	2.3
1	A	18	LYS	2.3
1	D	425	PRO	2.3
1	B	41	ARG	2.3
1	B	301	ASP	2.3
1	B	35	GLY	2.3
1	A	38	GLU	2.3
1	B	36	VAL	2.2
1	C	35	GLY	2.2
1	D	416	GLU	2.2
1	D	422	ALA	2.1
1	C	37	ASP	2.1
1	D	94	LEU	2.1
1	C	42	ALA	2.1
1	A	420	LEU	2.0
1	D	20	THR	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(Å <sup>2</sup> )	Q<0.9
3	SO4	D	801	5/5	0.90	0.18	90,95,95,95	5
3	SO4	C	603	5/5	0.92	0.20	45,56,57,57	5
3	SO4	A	501	5/5	0.93	0.15	89,95,95,95	5
3	SO4	A	503	5/5	0.94	0.16	43,56,57,57	5
3	SO4	B	702	5/5	0.94	0.16	44,56,57,57	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	B	701	5/5	0.94	0.17	83,87,87,87	0
2	TRP	D	800	15/15	0.95	0.19	72,72,74,74	0
3	SO4	A	703	5/5	0.95	0.16	42,54,56,56	5
3	SO4	A	502	5/5	0.95	0.14	45,58,59,60	5
3	SO4	D	802	5/5	0.95	0.14	41,53,55,55	5
2	TRP	A	500	15/15	0.96	0.21	56,56,62,62	0
3	SO4	C	601	5/5	0.96	0.14	48,60,62,62	5
2	TRP	C	600	15/15	0.96	0.23	49,50,53,53	0
3	SO4	C	602	5/5	0.96	0.14	38,52,53,53	5
2	TRP	B	700	15/15	0.97	0.20	53,54,61,61	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.