



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:11 am GMT

PDB ID : 3WFO  
Title : tRNA processing enzyme (apo form 1)  
Authors : Yamashita, S.; Takeshita, D.; Tomita, K.  
Deposited on : 2013-07-23  
Resolution : 3.40 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

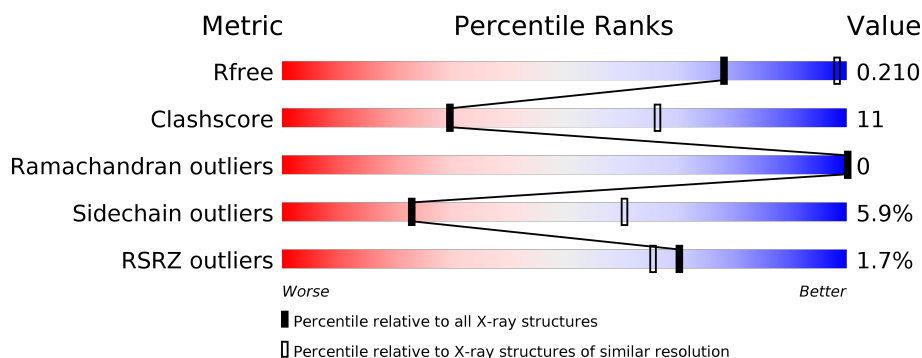
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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))
$R_{free}$	100719	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)

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	525	<div> <div>2%</div> <div>57% 21% 19%</div> </div>
1	B	525	<div> <div>63% 17% 19%</div> </div>
1	C	525	<div> <div>2%</div> <div>63% 16% 19%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	603	-	-	-	X
2	SO4	B	603	-	-	-	X
2	SO4	B	604	-	-	-	X
2	SO4	C	603	-	-	-	X

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10470 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 Poly A polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	0	0
			3469	2239	592	631	7			
1	B	426	Total	C	N	O	S	0	0	0
			3481	2244	596	634	7			
1	C	425	Total	C	N	O	S	0	0	0
			3465	2236	591	631	7			

There are 39 discrepancies between the modelled and reference sequences:

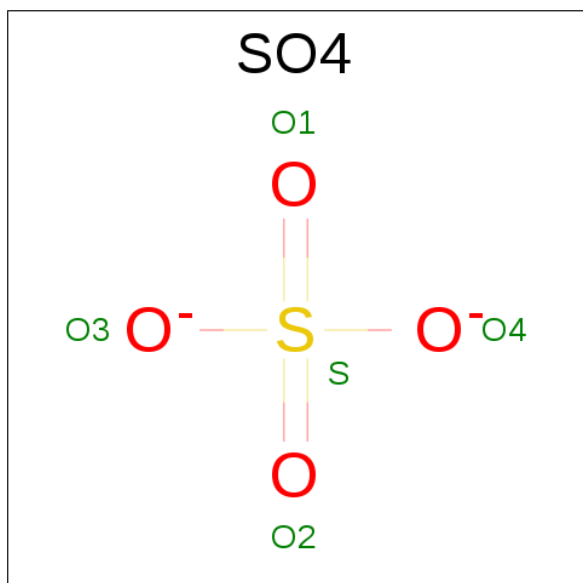
Chain	Residue	Modelled	Actual	Comment	Reference
A	513	LYS	-	EXPRESSION TAG	UNP O67911
A	514	LEU	-	EXPRESSION TAG	UNP O67911
A	515	ALA	-	EXPRESSION TAG	UNP O67911
A	516	ALA	-	EXPRESSION TAG	UNP O67911
A	517	ALA	-	EXPRESSION TAG	UNP O67911
A	518	LEU	-	EXPRESSION TAG	UNP O67911
A	519	GLU	-	EXPRESSION TAG	UNP O67911
A	520	HIS	-	EXPRESSION TAG	UNP O67911
A	521	HIS	-	EXPRESSION TAG	UNP O67911
A	522	HIS	-	EXPRESSION TAG	UNP O67911
A	523	HIS	-	EXPRESSION TAG	UNP O67911
A	524	HIS	-	EXPRESSION TAG	UNP O67911
A	525	HIS	-	EXPRESSION TAG	UNP O67911
B	513	LYS	-	EXPRESSION TAG	UNP O67911
B	514	LEU	-	EXPRESSION TAG	UNP O67911
B	515	ALA	-	EXPRESSION TAG	UNP O67911
B	516	ALA	-	EXPRESSION TAG	UNP O67911
B	517	ALA	-	EXPRESSION TAG	UNP O67911
B	518	LEU	-	EXPRESSION TAG	UNP O67911
B	519	GLU	-	EXPRESSION TAG	UNP O67911
B	520	HIS	-	EXPRESSION TAG	UNP O67911
B	521	HIS	-	EXPRESSION TAG	UNP O67911
B	522	HIS	-	EXPRESSION TAG	UNP O67911

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Chain	Residue	Modelled	Actual	Comment	Reference
B	523	HIS	-	EXPRESSION TAG	UNP O67911
B	524	HIS	-	EXPRESSION TAG	UNP O67911
B	525	HIS	-	EXPRESSION TAG	UNP O67911
C	513	LYS	-	EXPRESSION TAG	UNP O67911
C	514	LEU	-	EXPRESSION TAG	UNP O67911
C	515	ALA	-	EXPRESSION TAG	UNP O67911
C	516	ALA	-	EXPRESSION TAG	UNP O67911
C	517	ALA	-	EXPRESSION TAG	UNP O67911
C	518	LEU	-	EXPRESSION TAG	UNP O67911
C	519	GLU	-	EXPRESSION TAG	UNP O67911
C	520	HIS	-	EXPRESSION TAG	UNP O67911
C	521	HIS	-	EXPRESSION TAG	UNP O67911
C	522	HIS	-	EXPRESSION TAG	UNP O67911
C	523	HIS	-	EXPRESSION TAG	UNP O67911
C	524	HIS	-	EXPRESSION TAG	UNP O67911
C	525	HIS	-	EXPRESSION TAG	UNP O67911

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0

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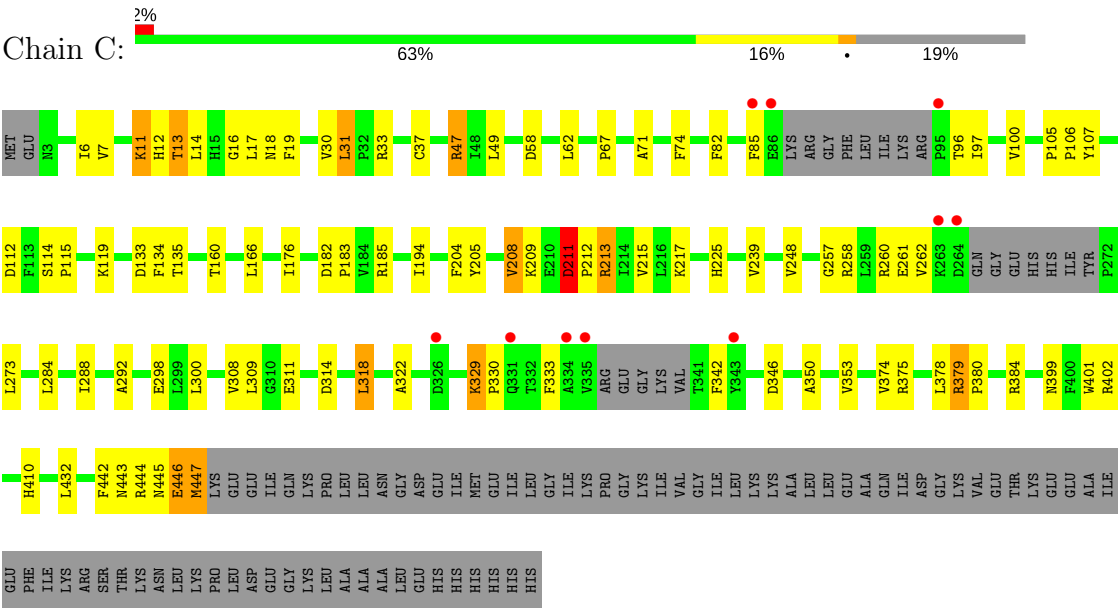
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0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



GLU	PHE	ILE	LYS	ARG	SER	THR	LYS	ASN	LEU	LYS	PRO	LEU	ASP	GLY	GLY	LYS	LEU	ALA	ALA	ALA	LEU	GLU	HIS	HIS	HIS	HIS	HIS
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● Molecule 1: Poly A polymerase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	177.48Å 327.77Å 78.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.88 – 3.40 19.88 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.88-3.40) 99.9 (19.88-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.96 (at 3.36Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1389)	Depositor
R, $R_{free}$	0.180 , 0.210 0.179 , 0.210	Depositor DCC
$R_{free}$ test set	1585 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	108.8	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 83.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10470	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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	0.31	0/3542	0.43	0/4772
1	B	0.25	0/3553	0.41	0/4786
1	C	0.28	1/3538 (0.0%)	0.45	1/4768 (0.0%)
All	All	0.28	1/10633 (0.0%)	0.43	1/14326 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	212	PRO	N-CD	5.16	1.55	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	211	ASP	C-N-CD	5.64	140.25	128.40

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	3469	0	3488	94	0
1	B	3481	0	3496	55	0
1	C	3465	0	3480	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	20	0	0	0	0
2	B	20	0	0	0	0
2	C	15	0	0	0	0
All	All	10470	0	10464	223	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 11.

All (223) 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:C:105:PRO:CG	1:C:106:PRO:HD3	1.64	1.26
1:A:147:LEU:O	1:A:149:ILE:HD13	1.47	1.14
1:C:105:PRO:HG2	1:C:106:PRO:CD	1.86	1.05
1:A:221:GLU:N	1:A:221:GLU:OE1	1.90	1.04
1:C:308:VAL:HG12	1:C:309:LEU:HD13	1.39	1.03
1:C:308:VAL:CG1	1:C:309:LEU:HD13	1.95	0.97
1:C:205:TYR:O	1:C:208:VAL:HG23	1.68	0.94
1:A:205:TYR:O	1:A:209:LYS:HG3	1.69	0.93
1:C:105:PRO:HG2	1:C:106:PRO:HD3	0.92	0.92
1:A:204:PHE:O	1:A:208:VAL:HG22	1.69	0.91
1:C:446:GLU:OE2	1:C:446:GLU:N	2.04	0.90
1:A:147:LEU:O	1:A:149:ILE:CD1	2.20	0.90
1:A:183:PRO:HG3	1:A:217:LYS:HB2	1.55	0.88
1:C:213:ARG:HG2	1:C:213:ARG:HH11	1.41	0.85
1:A:204:PHE:O	1:A:208:VAL:CG2	2.24	0.84
1:C:204:PHE:O	1:C:208:VAL:HG22	1.76	0.84
1:A:228:PHE:CE1	1:A:320:TRP:NE1	2.50	0.79
1:A:227:LEU:HD12	1:A:320:TRP:CH2	2.17	0.79
1:C:445:ASN:HB3	1:C:446:GLU:OE2	1.83	0.79
1:C:105:PRO:CD	1:C:106:PRO:HD3	2.15	0.77
1:A:227:LEU:HD12	1:A:320:TRP:HH2	1.49	0.76
1:C:211:ASP:N	1:C:211:ASP:OD1	2.20	0.74
1:C:105:PRO:CG	1:C:106:PRO:CD	2.56	0.74
1:C:183:PRO:HG3	1:C:217:LYS:HB2	1.70	0.74
1:A:5:GLU:HG2	1:B:7:VAL:HG22	1.71	0.72
1:A:225:HIS:NE2	1:A:311:GLU:OE2	2.22	0.72
1:A:307:ARG:NH2	1:A:310:GLY:O	2.23	0.71
1:C:205:TYR:HA	1:C:208:VAL:CG2	2.21	0.69
1:C:225:HIS:NE2	1:C:311:GLU:OE1	2.27	0.68
1:A:346:ASP:OD1	1:A:346:ASP:N	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:GLU:OE2	1:A:359:ARG:NH2	2.27	0.67
1:B:183:PRO:HG3	1:B:217:LYS:HB2	1.77	0.67
1:A:149:ILE:N	1:A:149:ILE:HD13	2.10	0.67
1:C:67:PRO:HG2	1:C:115:PRO:HG3	1.77	0.67
1:A:182:ASP:OD2	1:A:222:ARG:NH2	2.24	0.66
1:A:227:LEU:CD1	1:A:320:TRP:HH2	2.08	0.66
1:C:49:LEU:HD21	1:C:166:LEU:HD22	1.78	0.65
1:B:133:ASP:HB3	1:B:185:ARG:HD3	1.78	0.65
1:B:206:GLU:O	1:B:210:GLU:HG3	1.97	0.65
1:A:220:VAL:HG11	1:A:361:ARG:HG3	1.80	0.64
1:B:399:ASN:OD1	1:B:402:ARG:NH2	2.31	0.63
1:B:211:ASP:OD1	1:B:211:ASP:N	2.32	0.62
1:A:148:SER:OG	1:A:152:LYS:HG2	2.00	0.61
1:C:133:ASP:HB3	1:C:185:ARG:HD3	1.83	0.60
1:B:284:LEU:HD21	1:B:318:LEU:HD22	1.84	0.60
1:A:237:HIS:ND1	1:A:285:GLU:OE1	2.30	0.60
1:B:225:HIS:NE2	1:B:311:GLU:OE1	2.35	0.60
1:A:163:ILE:HD12	1:B:6:ILE:HD12	1.83	0.60
1:A:182:ASP:CG	1:A:222:ARG:HH22	2.04	0.60
1:B:152:LYS:O	1:B:153:GLN:HG3	2.01	0.60
1:A:220:VAL:CG1	1:A:361:ARG:HG3	2.32	0.59
1:A:205:TYR:O	1:A:208:VAL:HG23	2.03	0.59
1:A:30:VAL:HG12	1:A:70:LEU:HD12	1.83	0.59
1:A:353:VAL:HG21	1:A:374:VAL:HG21	1.84	0.59
1:A:7:VAL:HG13	1:B:155:ILE:HD11	1.85	0.59
1:B:284:LEU:HD22	1:B:322:ALA:HB2	1.85	0.59
1:C:105:PRO:CD	1:C:106:PRO:CD	2.81	0.59
1:C:11:LYS:O	1:C:12:HIS:HB2	2.02	0.59
1:C:353:VAL:HG21	1:C:374:VAL:HG21	1.84	0.59
1:A:284:LEU:HD21	1:A:318:LEU:HD22	1.85	0.58
1:A:215:VAL:HG21	1:A:248:VAL:HG13	1.86	0.58
1:A:205:TYR:HA	1:A:208:VAL:HG23	1.85	0.58
1:C:284:LEU:HD21	1:C:318:LEU:HD22	1.86	0.58
1:A:220:VAL:HG12	1:A:221:GLU:OE1	2.04	0.58
1:A:284:LEU:HD22	1:A:322:ALA:HB2	1.85	0.58
1:C:273:LEU:HD21	1:C:329:LYS:CD	2.33	0.58
1:C:308:VAL:HG13	1:C:309:LEU:HD13	1.85	0.58
1:A:104:LEU:HD23	1:A:106:PRO:HD2	1.86	0.57
1:A:227:LEU:CD1	1:A:320:TRP:CH2	2.85	0.57
1:C:183:PRO:HB2	1:C:215:VAL:HA	1.87	0.57
1:C:442:PHE:O	1:C:445:ASN:O	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ALA:O	1:A:223:ILE:HG12	2.04	0.57
1:A:204:PHE:O	1:A:208:VAL:HG23	2.05	0.57
1:A:292:ALA:HA	1:A:300:LEU:HD11	1.87	0.57
1:B:205:TYR:O	1:B:209:LYS:HG3	2.05	0.56
1:C:284:LEU:HD22	1:C:322:ALA:HB2	1.85	0.56
1:B:274:ASP:OD1	1:B:274:ASP:N	2.38	0.56
1:B:406:ASP:N	1:B:406:ASP:OD1	2.31	0.56
1:C:213:ARG:HG2	1:C:213:ARG:NH1	2.15	0.56
1:C:273:LEU:C	1:C:273:LEU:HD13	2.26	0.56
1:A:205:TYR:C	1:A:208:VAL:HG23	2.25	0.55
1:A:318:LEU:HG	1:A:410:HIS:HB3	1.88	0.55
1:A:205:TYR:CA	1:A:208:VAL:HG23	2.35	0.55
1:A:206:GLU:O	1:A:210:GLU:HG3	2.07	0.55
1:A:183:PRO:HB2	1:A:215:VAL:HA	1.87	0.55
1:A:399:ASN:OD1	1:A:402:ARG:NH2	2.40	0.55
1:B:237:HIS:ND1	1:B:285:GLU:OE2	2.35	0.55
1:B:308:VAL:HG12	1:B:309:LEU:HD13	1.88	0.55
1:C:133:ASP:OD1	1:C:134:PHE:N	2.39	0.55
1:A:49:LEU:HD21	1:A:166:LEU:HD22	1.88	0.54
1:A:406:ASP:N	1:A:406:ASP:OD1	2.32	0.54
1:A:47:ARG:NH1	1:A:51:GLU:O	2.40	0.54
1:B:292:ALA:HA	1:B:300:LEU:HD11	1.89	0.54
1:A:210:GLU:HB2	1:A:211:ASP:OD1	2.07	0.54
1:C:292:ALA:HA	1:C:300:LEU:HD11	1.90	0.54
1:B:183:PRO:HB2	1:B:215:VAL:HA	1.89	0.54
1:A:384:ARG:HD3	1:A:432:LEU:HB2	1.89	0.54
1:C:273:LEU:HD13	1:C:273:LEU:O	2.08	0.54
1:A:104:LEU:HD22	1:A:107:TYR:H	1.73	0.53
1:A:254:PRO:HD2	1:A:359:ARG:HH12	1.72	0.53
1:C:309:LEU:HD12	1:C:309:LEU:N	2.22	0.53
1:A:205:TYR:HA	1:A:208:VAL:CG2	2.38	0.53
1:A:259:LEU:HD21	1:A:327:ILE:HD12	1.89	0.53
1:B:215:VAL:HG21	1:B:248:VAL:HG13	1.91	0.53
1:C:16:GLY:O	1:C:19:PHE:N	2.40	0.53
1:C:205:TYR:C	1:C:208:VAL:HG23	2.28	0.53
1:C:135:THR:HG22	1:C:160:THR:HB	1.90	0.52
1:C:318:LEU:HG	1:C:410:HIS:HB3	1.90	0.52
1:A:250:GLU:OE2	1:A:260:ARG:NH2	2.40	0.52
1:C:215:VAL:HG21	1:C:248:VAL:HG13	1.91	0.52
1:A:218:SER:OG	1:A:223:ILE:HD11	2.10	0.52
1:A:359:ARG:HG2	1:A:360:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ARG:HG2	1:A:226:GLU:OE2	2.10	0.51
1:C:309:LEU:CD1	1:C:309:LEU:N	2.73	0.51
1:A:372:LYS:HG2	1:A:407:ILE:HD13	1.91	0.51
1:C:213:ARG:CG	1:C:213:ARG:HH11	2.15	0.51
1:A:133:ASP:N	1:A:133:ASP:OD1	2.44	0.50
1:B:135:THR:HG22	1:B:160:THR:HB	1.93	0.50
1:B:62:LEU:HD23	1:B:114:SER:HB2	1.93	0.50
1:C:14:LEU:O	1:C:19:PHE:CE2	2.64	0.50
1:A:57:ILE:HD12	1:A:109:TYR:CE2	2.47	0.50
1:C:298:GLU:OE2	1:C:444:ARG:NH1	2.42	0.50
1:A:309:LEU:HD11	1:A:363:GLY:H	1.77	0.49
1:A:354:ARG:NH1	1:A:368:GLU:OE1	2.46	0.49
1:C:273:LEU:HD21	1:C:329:LYS:HD3	1.92	0.49
1:B:334:ALA:HB2	1:B:341:THR:HA	1.95	0.49
1:C:384:ARG:HD3	1:C:432:LEU:HB2	1.94	0.49
1:A:67:PRO:HG2	1:A:115:PRO:HG3	1.93	0.49
1:C:14:LEU:O	1:C:19:PHE:HE2	1.96	0.49
1:B:318:LEU:HG	1:B:410:HIS:HB3	1.95	0.48
1:A:211:ASP:OD1	1:A:211:ASP:N	2.46	0.48
1:C:346:ASP:OD1	1:C:346:ASP:N	2.46	0.48
1:A:149:ILE:N	1:A:149:ILE:CD1	2.73	0.48
1:A:102:LEU:HB3	1:A:109:TYR:HB2	1.95	0.48
1:B:49:LEU:HD21	1:B:166:LEU:HD22	1.95	0.48
1:C:213:ARG:CG	1:C:213:ARG:NH1	2.73	0.48
1:C:399:ASN:OD1	1:C:402:ARG:NH2	2.47	0.48
1:C:176:ILE:HD12	1:C:176:ILE:H	1.79	0.48
1:B:67:PRO:HG2	1:B:115:PRO:HG3	1.95	0.47
1:C:47:ARG:HA	1:C:47:ARG:HD3	1.54	0.47
1:C:13:THR:O	1:C:18:ASN:ND2	2.30	0.47
1:A:135:THR:HG22	1:A:160:THR:HB	1.96	0.47
1:A:326:ASP:OD1	1:A:377:HIS:NE2	2.48	0.47
1:A:6:ILE:HG22	1:B:156:VAL:HG22	1.97	0.47
1:B:372:LYS:HG2	1:B:407:ILE:HD13	1.98	0.46
1:B:384:ARG:HD3	1:B:432:LEU:HB2	1.97	0.46
1:B:57:ILE:HD12	1:B:109:TYR:CE2	2.50	0.46
1:A:62:LEU:HD23	1:A:114:SER:HB2	1.97	0.46
1:B:133:ASP:OD1	1:B:134:PHE:N	2.43	0.46
1:C:97:ILE:HD11	1:C:112:ASP:HB3	1.97	0.46
1:A:207:PHE:CD1	1:A:207:PHE:C	2.87	0.46
1:C:288:ILE:HD11	1:C:318:LEU:HD13	1.97	0.46
1:C:258:ARG:O	1:C:261:GLU:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:ASP:OD1	1:C:314:ASP:N	2.45	0.45
1:B:308:VAL:O	1:B:309:LEU:HB2	2.16	0.45
1:B:173:PRO:HB3	1:B:179:LEU:HD21	1.98	0.45
1:B:27:VAL:HA	1:B:30:VAL:HG12	1.97	0.45
1:B:120:ASP:HB3	1:B:123:LYS:HB3	1.98	0.45
1:C:96:THR:OG1	1:C:115:PRO:HG2	2.16	0.45
1:A:185:ARG:HA	1:A:185:ARG:HD2	1.78	0.45
1:A:227:LEU:HD12	1:A:320:TRP:CZ2	2.51	0.45
1:B:353:VAL:HG21	1:B:374:VAL:HG21	1.99	0.45
1:B:442:PHE:O	1:B:447:MET:HB2	2.17	0.45
1:C:273:LEU:C	1:C:273:LEU:CD1	2.85	0.45
1:A:104:LEU:CD2	1:A:106:PRO:HD2	2.45	0.45
1:C:31:LEU:HD11	1:C:37:CYS:HB2	1.99	0.45
1:A:220:VAL:HG13	1:A:221:GLU:N	2.33	0.44
1:A:347:LYS:HE2	1:A:375:ARG:NH2	2.33	0.44
1:C:217:LYS:HE2	1:C:217:LYS:HB3	1.84	0.44
1:C:71:ALA:HB1	1:C:100:VAL:HG23	2.00	0.44
1:C:401:TRP:CE2	1:C:443:ASN:HB2	2.53	0.44
1:C:62:LEU:HD23	1:C:114:SER:HB3	1.99	0.44
1:B:446:GLU:H	1:B:446:GLU:HG2	1.64	0.43
1:C:205:TYR:CA	1:C:208:VAL:CG2	2.94	0.43
1:A:154:THR:O	1:B:4:ILE:HD12	2.18	0.43
1:B:30:VAL:HG11	1:B:74:PHE:HB2	2.00	0.43
1:C:11:LYS:HE2	1:C:11:LYS:HB3	1.72	0.43
1:B:31:LEU:HD23	1:B:32:PRO:HD2	2.01	0.43
1:B:377:HIS:HA	1:B:411:LEU:HD11	2.01	0.43
1:A:258:ARG:O	1:A:261:GLU:HG2	2.18	0.43
1:B:194:ILE:HG13	1:B:239:VAL:HG22	2.00	0.43
1:A:227:LEU:HD22	1:A:227:LEU:HA	1.87	0.42
1:B:188:ARG:HG3	1:B:191:ARG:HH21	1.84	0.42
1:A:133:ASP:HB3	1:A:185:ARG:HG3	2.01	0.42
1:A:379:ARG:HB3	1:A:380:PRO:HD3	2.01	0.42
1:A:329:LYS:HE3	1:A:342:PHE:CD1	2.55	0.42
1:A:148:SER:CB	1:A:152:LYS:HG2	2.49	0.42
1:A:47:ARG:HA	1:A:47:ARG:HD3	1.50	0.42
1:B:105:PRO:HG2	1:B:106:PRO:HD3	2.02	0.42
1:C:350:ALA:HB2	1:C:375:ARG:HB2	2.01	0.42
1:C:194:ILE:HG13	1:C:239:VAL:HG22	2.01	0.42
1:C:257:GLY:O	1:C:260:ARG:HG2	2.19	0.42
1:A:308:VAL:HG21	1:A:317:LEU:HD11	2.02	0.42
1:A:220:VAL:CG1	1:A:221:GLU:N	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:VAL:HG11	1:C:74:PHE:HB2	2.02	0.42
1:A:120:ASP:HB3	1:A:123:LYS:HE3	2.01	0.42
1:B:182:ASP:HB3	1:B:185:ARG:HD2	2.02	0.42
1:C:114:SER:HA	1:C:115:PRO:HD3	1.85	0.42
1:C:446:GLU:O	1:C:447:MET:SD	2.78	0.41
1:A:228:PHE:O	1:A:231:MET:N	2.53	0.41
1:B:379:ARG:HB3	1:B:380:PRO:HD3	2.02	0.41
1:C:106:PRO:HB2	1:C:107:TYR:CD2	2.55	0.41
1:A:255:GLU:CD	1:A:359:ARG:HH22	2.23	0.41
1:C:16:GLY:O	1:C:17:LEU:C	2.57	0.41
1:C:6:ILE:HG22	1:C:7:VAL:N	2.35	0.41
1:A:323:LEU:HD23	1:A:323:LEU:HA	1.87	0.41
1:B:323:LEU:HA	1:B:323:LEU:HD23	1.91	0.41
1:B:327:ILE:HG23	1:B:352:ILE:HD12	2.01	0.41
1:C:208:VAL:O	1:C:209:LYS:C	2.58	0.41
1:B:85:PHE:CG	1:B:86:GLU:N	2.89	0.41
1:B:183:PRO:HB3	1:B:214:ILE:HG13	2.02	0.41
1:B:139:ILE:HG23	1:B:158:ASP:HB3	2.01	0.41
1:C:182:ASP:HB3	1:C:185:ARG:HD2	2.00	0.41
1:C:18:ASN:O	1:C:47:ARG:HG3	2.20	0.41
1:B:401:TRP:CE2	1:B:443:ASN:HB2	2.56	0.41
1:B:314:ASP:N	1:B:314:ASP:OD1	2.46	0.41
1:C:379:ARG:HB3	1:C:380:PRO:HD3	2.03	0.41
1:A:274:ASP:OD1	1:A:275:GLU:N	2.54	0.41
1:C:262:VAL:HG21	1:C:330:PRO:HA	2.03	0.41
1:A:68:VAL:HG13	1:A:82:PHE:HZ	1.86	0.41
1:A:329:LYS:N	1:A:330:PRO:HD2	2.35	0.40
1:A:60:ASP:OD2	1:A:132:ARG:NH2	2.54	0.40
1:B:125:LEU:O	1:B:129:LEU:HG	2.22	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	417/525 (79%)	415 (100%)	2 (0%)	0	100	100
1	B	418/525 (80%)	417 (100%)	1 (0%)	0	100	100
1	C	417/525 (79%)	415 (100%)	2 (0%)	0	100	100
All	All	1252/1575 (80%)	1247 (100%)	5 (0%)	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	370/454 (82%)	343 (93%)	27 (7%)	16	52
1	B	370/454 (82%)	352 (95%)	18 (5%)	29	66
1	C	369/454 (81%)	349 (95%)	20 (5%)	26	63
All	All	1109/1362 (81%)	1044 (94%)	65 (6%)	23	60

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	4	ILE
1	A	8	SER
1	A	12	HIS
1	A	13	THR
1	A	47	ARG
1	A	53	VAL
1	A	104	LEU
1	A	149	ILE
1	A	185	ARG
1	A	186	VAL
1	A	203	ASP
1	A	207	PHE
1	A	208	VAL
1	A	211	ASP

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Mol	Chain	Res	Type
1	A	227	LEU
1	A	262	VAL
1	A	264	ASP
1	A	277	THR
1	A	318	LEU
1	A	343	TYR
1	A	346	ASP
1	A	360	LEU
1	A	377	HIS
1	A	378	LEU
1	A	406	ASP
1	A	445	ASN
1	B	4	ILE
1	B	6	ILE
1	B	12	HIS
1	B	31	LEU
1	B	33	ARG
1	B	86	GLU
1	B	152	LYS
1	B	154	THR
1	B	176	ILE
1	B	186	VAL
1	B	211	ASP
1	B	318	LEU
1	B	333	PHE
1	B	346	ASP
1	B	377	HIS
1	B	378	LEU
1	B	406	ASP
1	B	446	GLU
1	C	11	LYS
1	C	13	THR
1	C	31	LEU
1	C	33	ARG
1	C	47	ARG
1	C	58	ASP
1	C	82	PHE
1	C	85	PHE
1	C	119	LYS
1	C	208	VAL
1	C	211	ASP
1	C	213	ARG

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Mol	Chain	Res	Type
1	C	318	LEU
1	C	329	LYS
1	C	333	PHE
1	C	342	PHE
1	C	378	LEU
1	C	379	ARG
1	C	446	GLU
1	C	447	MET

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 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](#)

11 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	SO4	A	601	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	A	602	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	A	603	-	4,4,4	0.15	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	604	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	B	601	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	602	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	B	603	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	B	604	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	C	601	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	C	602	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	C	603	-	4,4,4	0.15	0	6,6,6	0.06	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	SO4	A	601	-	-	0/0/0/0	0/0/0/0
2	SO4	A	602	-	-	0/0/0/0	0/0/0/0
2	SO4	A	603	-	-	0/0/0/0	0/0/0/0
2	SO4	A	604	-	-	0/0/0/0	0/0/0/0
2	SO4	B	601	-	-	0/0/0/0	0/0/0/0
2	SO4	B	602	-	-	0/0/0/0	0/0/0/0
2	SO4	B	603	-	-	0/0/0/0	0/0/0/0
2	SO4	B	604	-	-	0/0/0/0	0/0/0/0
2	SO4	C	601	-	-	0/0/0/0	0/0/0/0
2	SO4	C	602	-	-	0/0/0/0	0/0/0/0
2	SO4	C	603	-	-	0/0/0/0	0/0/0/0

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.

No monomer is involved in short contacts.

## 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, 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	425/525 (80%)	-0.43	5 (1%) 79 75	63, 104, 162, 204	0
1	B	426/525 (81%)	-0.35	7 (1%) 72 67	70, 115, 179, 228	0
1	C	425/525 (80%)	-0.27	10 (2%) 59 55	76, 118, 189, 246	0
All	All	1276/1575 (81%)	-0.35	22 (1%) 70 66	63, 113, 179, 246	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	335	VAL	7.3
1	C	264	ASP	4.2
1	C	85	PHE	4.0
1	C	86	GLU	3.8
1	A	343	TYR	3.8
1	C	343	TYR	3.3
1	B	3	ASN	3.1
1	C	334	ALA	3.1
1	C	326	ASP	3.0
1	B	334	ALA	2.8
1	A	263	LYS	2.6
1	A	344	GLU	2.6
1	C	263	LYS	2.6
1	A	95	PRO	2.5
1	B	326	ASP	2.4
1	A	119	LYS	2.3
1	C	95	PRO	2.2
1	C	331	GLN	2.2
1	B	449	GLU	2.2
1	B	85	PHE	2.1
1	B	263	LYS	2.0
1	B	343	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. 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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	603	5/5	0.89	0.39	10.77	155,170,173,180	0
2	SO4	B	603	5/5	0.80	0.56	6.50	177,182,189,195	0
2	SO4	C	603	5/5	0.86	0.42	6.34	172,176,184,187	0
2	SO4	B	604	5/5	0.87	0.29	2.72	174,184,187,189	0
2	SO4	A	604	5/5	0.88	0.24	1.21	165,173,176,178	0
2	SO4	A	601	5/5	0.97	0.09	-2.52	116,128,137,141	0
2	SO4	B	601	5/5	0.95	0.09	-2.93	120,127,142,143	0
2	SO4	C	601	5/5	0.96	0.10	-2.96	117,128,142,147	0
2	SO4	B	602	5/5	0.88	0.51	-	189,189,199,210	0
2	SO4	C	602	5/5	0.83	0.35	-	179,187,191,202	0
2	SO4	A	602	5/5	0.92	0.27	-	140,142,159,166	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.