



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:38 PM GMT

PDB ID : 1XZP  
Title : Structure of the GTP-binding protein TrmE from *Thermotoga maritima*  
Authors : Scrima, A.; Vetter, I.R.; Armengod, M.E.; Wittinghofer, A.  
Deposited on : 2004-11-12  
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  
<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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

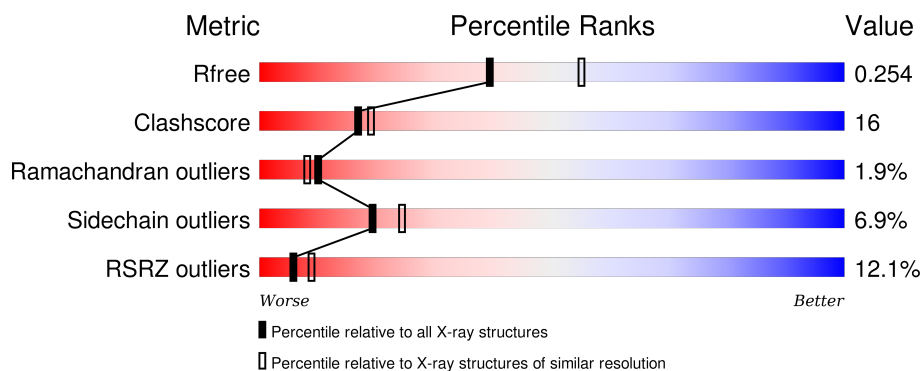
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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	482	
2	B	150	

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
3	SO4	A	1005	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4708 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 Probable tRNA modification GTPase trmE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	0	0
			3554	2235	625	683	11			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-31	MET	-	EXPRESSION TAG	UNP Q9WYA4
A	-30	GLY	-	EXPRESSION TAG	UNP Q9WYA4
A	-29	SER	-	EXPRESSION TAG	UNP Q9WYA4
A	-28	SER	-	EXPRESSION TAG	UNP Q9WYA4
A	-27	HIS	-	EXPRESSION TAG	UNP Q9WYA4
A	-26	HIS	-	EXPRESSION TAG	UNP Q9WYA4
A	-25	HIS	-	EXPRESSION TAG	UNP Q9WYA4
A	-24	HIS	-	EXPRESSION TAG	UNP Q9WYA4
A	-23	HIS	-	EXPRESSION TAG	UNP Q9WYA4
A	-22	HIS	-	EXPRESSION TAG	UNP Q9WYA4
A	-21	SER	-	EXPRESSION TAG	UNP Q9WYA4
A	-20	SER	-	EXPRESSION TAG	UNP Q9WYA4
A	-19	GLY	-	EXPRESSION TAG	UNP Q9WYA4
A	-18	LEU	-	EXPRESSION TAG	UNP Q9WYA4
A	-17	VAL	-	EXPRESSION TAG	UNP Q9WYA4
A	-16	PRO	-	EXPRESSION TAG	UNP Q9WYA4
A	-15	ARG	-	EXPRESSION TAG	UNP Q9WYA4
A	-14	GLY	-	EXPRESSION TAG	UNP Q9WYA4
A	-13	SER	-	EXPRESSION TAG	UNP Q9WYA4
A	-12	HIS	-	EXPRESSION TAG	UNP Q9WYA4
A	-11	TRP	-	EXPRESSION TAG	UNP Q9WYA4
A	-10	GLY	-	EXPRESSION TAG	UNP Q9WYA4
A	-9	SER	-	EXPRESSION TAG	UNP Q9WYA4
A	-8	PRO	-	EXPRESSION TAG	UNP Q9WYA4
A	-7	ASN	-	EXPRESSION TAG	UNP Q9WYA4
A	-6	SER	-	EXPRESSION TAG	UNP Q9WYA4
A	-5	SER	-	EXPRESSION TAG	UNP Q9WYA4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	SER	-	EXPRESSION TAG	UNP Q9WYA4
A	-3	VAL	-	EXPRESSION TAG	UNP Q9WYA4
A	-2	ASP	-	EXPRESSION TAG	UNP Q9WYA4
A	-1	LYS	-	EXPRESSION TAG	UNP Q9WYA4
A	0	LEU	-	EXPRESSION TAG	UNP Q9WYA4

- Molecule 2 is a protein called Probable tRNA modification GTPase trmE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	131	Total	C	N	O	S	0	0	0
			992	633	175	179	5			

There are 32 discrepancies between the modelled and reference sequences:

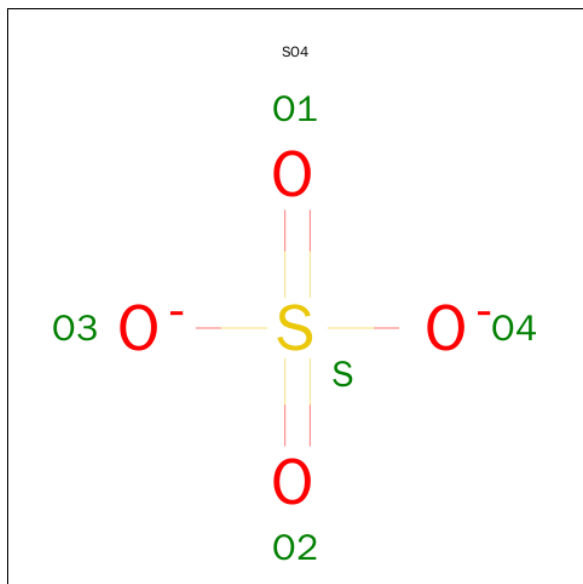
Chain	Residue	Modelled	Actual	Comment	Reference
B	-31	MET	-	EXPRESSION TAG	UNP Q9WYA4
B	-30	GLY	-	EXPRESSION TAG	UNP Q9WYA4
B	-29	SER	-	EXPRESSION TAG	UNP Q9WYA4
B	-28	SER	-	EXPRESSION TAG	UNP Q9WYA4
B	-27	HIS	-	EXPRESSION TAG	UNP Q9WYA4
B	-26	HIS	-	EXPRESSION TAG	UNP Q9WYA4
B	-25	HIS	-	EXPRESSION TAG	UNP Q9WYA4
B	-24	HIS	-	EXPRESSION TAG	UNP Q9WYA4
B	-23	HIS	-	EXPRESSION TAG	UNP Q9WYA4
B	-22	HIS	-	EXPRESSION TAG	UNP Q9WYA4
B	-21	SER	-	EXPRESSION TAG	UNP Q9WYA4
B	-20	SER	-	EXPRESSION TAG	UNP Q9WYA4
B	-19	GLY	-	EXPRESSION TAG	UNP Q9WYA4
B	-18	LEU	-	EXPRESSION TAG	UNP Q9WYA4
B	-17	VAL	-	EXPRESSION TAG	UNP Q9WYA4
B	-16	PRO	-	EXPRESSION TAG	UNP Q9WYA4
B	-15	ARG	-	EXPRESSION TAG	UNP Q9WYA4
B	-14	GLY	-	EXPRESSION TAG	UNP Q9WYA4
B	-13	SER	-	EXPRESSION TAG	UNP Q9WYA4
B	-12	HIS	-	EXPRESSION TAG	UNP Q9WYA4
B	-11	TRP	-	EXPRESSION TAG	UNP Q9WYA4
B	-10	GLY	-	EXPRESSION TAG	UNP Q9WYA4
B	-9	SER	-	EXPRESSION TAG	UNP Q9WYA4
B	-8	PRO	-	EXPRESSION TAG	UNP Q9WYA4
B	-7	ASN	-	EXPRESSION TAG	UNP Q9WYA4
B	-6	SER	-	EXPRESSION TAG	UNP Q9WYA4
B	-5	SER	-	EXPRESSION TAG	UNP Q9WYA4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	SER	-	EXPRESSION TAG	UNP Q9WYA4
B	-3	VAL	-	EXPRESSION TAG	UNP Q9WYA4
B	-2	ASP	-	EXPRESSION TAG	UNP Q9WYA4
B	-1	LYS	-	EXPRESSION TAG	UNP Q9WYA4
B	0	LEU	-	EXPRESSION TAG	UNP Q9WYA4

- Molecule 3 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

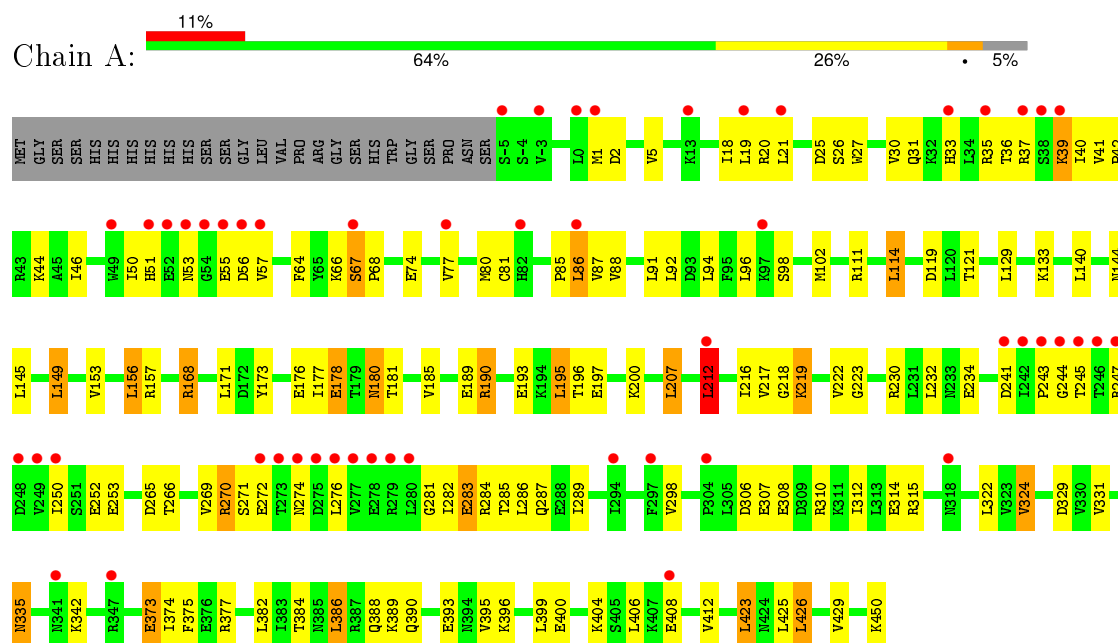
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	96	Total	O	0	0
			96	96		
4	B	41	Total	O	0	0
			41	41		

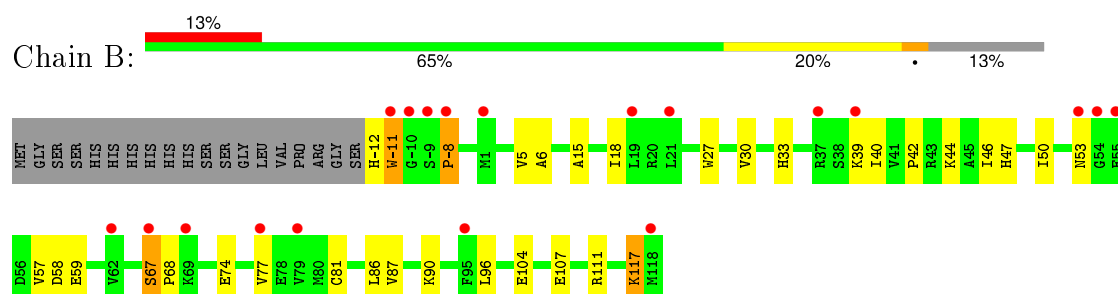
### 3 Residue-property plots [i](#)

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: Probable tRNA modification GTPase trmE



- Molecule 2: Probable tRNA modification GTPase trmE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.85Å 128.85Å 107.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.70 – 2.30 19.70 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.70-2.30) 99.8 (19.70-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.35 (at 2.30Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.226 , 0.252 0.229 , 0.254	Depositor DCC
$R_{free}$ test set	2236 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.9	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 63.5	EDS
Estimated twinning fraction	0.037 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 44730 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4708	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.33	0/3590	0.61	2/4829 (0.0%)
2	B	0.33	0/1012	0.68	1/1364 (0.1%)
All	All	0.33	0/4602	0.62	3/6193 (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	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	243	PRO	N-CA-CB	5.74	110.19	103.30
1	A	212	LEU	CA-CB-CG	5.63	128.25	115.30
2	B	-8	PRO	N-CA-CB	5.42	109.81	103.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	244	GLY	Mainchain

## 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	3554	0	3653	132	0
2	B	992	0	1011	23	0
3	A	15	0	0	1	0
3	B	10	0	0	0	0
4	A	96	0	0	3	0
4	B	41	0	0	0	0
All	All	4708	0	4664	151	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 16.

All (151) 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:314:GLU:HG2	1:A:342:LYS:HE3	1.47	0.95
1:A:230:ARG:HD2	1:A:234:GLU:OE2	1.70	0.92
1:A:232:LEU:CD2	1:A:269:VAL:HG21	2.09	0.82
1:A:40:ILE:H	1:A:40:ILE:HD12	1.44	0.82
1:A:384:THR:H	1:A:388:GLN:HE22	1.28	0.81
2:B:117:LYS:HA	2:B:117:LYS:HE2	1.63	0.81
1:A:232:LEU:HD22	1:A:269:VAL:HG21	1.66	0.78
1:A:395:VAL:HG21	1:A:426:LEU:HD13	1.66	0.78
1:A:102:MET:HE2	1:A:102:MET:HA	1.65	0.78
1:A:270:ARG:HH11	1:A:270:ARG:HB2	1.49	0.77
1:A:55:GLU:HB3	1:A:57:VAL:HG13	1.69	0.75
2:B:67:SER:HB3	2:B:68:PRO:HD3	1.69	0.74
1:A:265:ASP:OD2	1:A:269:VAL:HG22	1.88	0.73
1:A:282:ILE:O	1:A:286:LEU:HD23	1.88	0.73
1:A:384:THR:H	1:A:388:GLN:NE2	1.87	0.72
1:A:51:HIS:HB3	1:A:56:ASP:HA	1.70	0.72
1:A:18:ILE:HD11	2:B:18:ILE:HD11	1.73	0.70
1:A:450:LYS:HD2	2:B:15:ALA:HB1	1.73	0.70
1:A:92:LEU:HD11	1:A:102:MET:HE3	1.78	0.66
1:A:86:LEU:HD23	1:A:86:LEU:H	1.60	0.66
1:A:55:GLU:O	1:A:56:ASP:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ARG:NH1	1:A:270:ARG:HB2	2.11	0.65
2:B:50:ILE:O	2:B:57:VAL:HG22	1.97	0.65
1:A:314:GLU:HG2	1:A:342:LYS:CE	2.26	0.63
1:A:282:ILE:HD12	1:A:308:GLU:HG3	1.80	0.62
1:A:153:VAL:HG21	1:A:429:VAL:HG21	1.81	0.62
1:A:40:ILE:H	1:A:40:ILE:CD1	2.13	0.62
1:A:306:ASP:O	1:A:310:ARG:HG3	2.01	0.61
1:A:121:THR:HG21	1:A:149:LEU:HD13	1.82	0.61
1:A:33:HIS:O	1:A:50:ILE:HD12	2.00	0.61
1:A:18:ILE:CD1	2:B:18:ILE:HD11	2.30	0.61
1:A:50:ILE:O	1:A:50:ILE:HG23	2.01	0.60
1:A:329:ASP:OD1	1:A:331:VAL:HG12	2.02	0.60
1:A:272:GLU:H	1:A:272:GLU:CD	2.05	0.59
1:A:373:GLU:OE1	1:A:374:ILE:HG13	2.00	0.59
1:A:44:LYS:O	1:A:46:ILE:HG12	2.03	0.59
2:B:44:LYS:O	2:B:46:ILE:HG13	2.02	0.59
1:A:386:LEU:HD22	1:A:390:GLN:HG3	1.83	0.59
1:A:223:GLY:O	1:A:269:VAL:HA	2.03	0.59
1:A:86:LEU:HD23	1:A:86:LEU:N	2.18	0.58
1:A:216:ILE:O	1:A:266:THR:HB	2.03	0.58
1:A:171:LEU:HD11	1:A:412:VAL:HG23	1.86	0.58
1:A:92:LEU:HD11	1:A:102:MET:CE	2.34	0.57
1:A:180:ASN:C	1:A:180:ASN:HD22	2.07	0.57
1:A:40:ILE:HD12	1:A:40:ILE:N	2.15	0.56
1:A:177:ILE:HD12	1:A:177:ILE:N	2.20	0.56
1:A:185:VAL:O	1:A:189:GLU:HG3	2.06	0.56
1:A:133:LYS:HE2	1:A:253:GLU:OE1	2.06	0.56
1:A:67:SER:HB3	1:A:68:PRO:CD	2.36	0.55
2:B:30:VAL:HG21	2:B:77:VAL:HG11	1.87	0.55
1:A:86:LEU:H	1:A:86:LEU:CD2	2.21	0.54
1:A:219:LYS:HD2	4:A:1092:HOH:O	2.06	0.54
1:A:219:LYS:HE2	1:A:219:LYS:N	2.22	0.54
1:A:389:LYS:O	1:A:393:GLU:HG3	2.08	0.53
1:A:173:TYR:HB2	1:A:177:ILE:HD13	1.91	0.53
1:A:18:ILE:HG12	1:A:80:MET:HG2	1.89	0.53
1:A:298:VAL:HG22	1:A:324:VAL:HG13	1.91	0.53
1:A:81:CYS:SG	1:A:88:VAL:HG12	2.47	0.53
1:A:219:LYS:O	1:A:222:VAL:HG22	2.08	0.52
1:A:450:LYS:HD2	2:B:15:ALA:CB	2.39	0.52
1:A:39:LYS:O	1:A:41:VAL:HG23	2.09	0.52
1:A:270:ARG:HH11	1:A:270:ARG:CB	2.21	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:ASP:OD2	2:B:81:CYS:HB2	2.10	0.52
1:A:269:VAL:O	1:A:269:VAL:HG23	2.10	0.52
1:A:283:GLU:CD	1:A:283:GLU:H	2.13	0.52
2:B:-12:HIS:O	2:B:-11:TRP:O	2.28	0.52
1:A:86:LEU:HG	1:A:87:VAL:HG23	1.92	0.52
1:A:94:LEU:O	1:A:98:SER:HB2	2.10	0.52
1:A:168:ARG:O	1:A:168:ARG:HG3	2.09	0.51
1:A:271:SER:HB2	1:A:272:GLU:OE2	2.09	0.51
1:A:33:HIS:HB3	1:A:51:HIS:O	2.10	0.51
1:A:298:VAL:HG22	1:A:324:VAL:CG1	2.41	0.51
1:A:250:ILE:HD12	1:A:250:ILE:N	2.27	0.50
1:A:67:SER:CB	1:A:68:PRO:CD	2.90	0.50
1:A:33:HIS:HB2	1:A:50:ILE:HD11	1.93	0.49
1:A:21:LEU:HB2	1:A:77:VAL:HG12	1.93	0.49
1:A:335:ASN:HD22	1:A:335:ASN:C	2.13	0.49
1:A:181:THR:HG23	1:A:406:LEU:HB3	1.94	0.49
2:B:47:HIS:HE1	2:B:59:GLU:OE2	1.95	0.49
1:A:270:ARG:HD2	1:A:272:GLU:OE1	2.13	0.48
1:A:396:LYS:O	1:A:400:GLU:HG3	2.13	0.48
1:A:33:HIS:C	1:A:50:ILE:HD12	2.34	0.48
1:A:218:GLY:C	1:A:219:LYS:HE2	2.34	0.48
1:A:85:PRO:O	1:A:88:VAL:HG22	2.14	0.48
1:A:404:LYS:O	1:A:408:GLU:HG3	2.13	0.48
1:A:133:LYS:NZ	4:A:1027:HOH:O	2.43	0.47
2:B:67:SER:HA	2:B:74:GLU:C	2.34	0.47
1:A:1:MET:CG	1:A:111:ARG:NH2	2.77	0.47
1:A:1:MET:HG2	1:A:111:ARG:NH2	2.30	0.47
1:A:270:ARG:HG3	1:A:271:SER:N	2.29	0.47
1:A:129:LEU:C	1:A:129:LEU:HD23	2.35	0.47
1:A:27:TRP:O	1:A:30:VAL:HG12	2.15	0.47
1:A:35:ARG:HB2	1:A:51:HIS:HD2	1.80	0.46
1:A:21:LEU:HB2	1:A:77:VAL:CG1	2.44	0.46
1:A:286:LEU:HD12	1:A:315:ARG:HG2	1.98	0.46
1:A:171:LEU:CD1	1:A:412:VAL:HG23	2.46	0.46
2:B:27:TRP:HH2	2:B:42:PRO:HG3	1.80	0.46
2:B:67:SER:CB	2:B:68:PRO:HD3	2.42	0.46
2:B:58:ASP:HB2	2:B:87:VAL:CG2	2.46	0.46
1:A:377:ARG:NH2	4:A:1082:HOH:O	2.48	0.46
1:A:19:LEU:HD12	1:A:19:LEU:HA	1.80	0.46
2:B:40:ILE:HA	2:B:46:ILE:CD1	2.46	0.46
1:A:42:PRO:HA	1:A:64:PHE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HG3	1:A:2:ASP:N	2.31	0.45
1:A:31:GLN:OE1	1:A:40:ILE:HG12	2.16	0.45
2:B:58:ASP:HB2	2:B:87:VAL:HG21	1.97	0.45
2:B:86:LEU:HD11	2:B:90:LYS:HE2	1.99	0.45
1:A:217:VAL:HG11	1:A:312:ILE:HD13	1.98	0.45
1:A:86:LEU:HG	1:A:87:VAL:H	1.81	0.45
1:A:286:LEU:HD12	1:A:315:ARG:NH2	2.32	0.45
1:A:35:ARG:HB2	1:A:51:HIS:CD2	2.52	0.44
1:A:284:ARG:HH11	1:A:284:ARG:HG2	1.81	0.44
1:A:36:THR:OG1	1:A:37:ARG:N	2.49	0.44
2:B:104:GLU:HG3	2:B:107:GLU:OE1	2.18	0.44
1:A:196:THR:HG22	1:A:200:LYS:HE3	1.99	0.44
1:A:190:ARG:O	1:A:190:ARG:NE	2.51	0.44
1:A:285:THR:O	1:A:289:ILE:HG13	2.17	0.44
1:A:87:VAL:O	1:A:91:LEU:HB2	2.17	0.44
1:A:281:GLY:HA3	1:A:283:GLU:OE2	2.17	0.43
1:A:5:VAL:HG13	1:A:102:MET:CE	2.49	0.43
1:A:156:LEU:HD21	1:A:195:LEU:HG	2.00	0.43
1:A:375:PHE:CD1	1:A:375:PHE:C	2.91	0.43
1:A:144:ASN:ND2	1:A:149:LEU:H	2.17	0.43
1:A:25:ASP:O	1:A:26:SER:C	2.56	0.43
1:A:1:MET:HG2	1:A:111:ARG:HH21	1.84	0.43
1:A:196:THR:O	1:A:200:LYS:HG3	2.19	0.43
1:A:207:LEU:HG	1:A:212:LEU:HD22	2.01	0.43
1:A:96:LEU:HD21	1:A:102:MET:HE3	2.01	0.42
1:A:331:VAL:HG13	1:A:331:VAL:O	2.19	0.42
1:A:86:LEU:HG	1:A:87:VAL:N	2.34	0.42
1:A:335:ASN:ND2	1:A:335:ASN:C	2.73	0.42
2:B:40:ILE:HA	2:B:46:ILE:HD11	2.01	0.42
1:A:283:GLU:O	1:A:287:GLN:HG3	2.19	0.42
1:A:193:GLU:O	1:A:197:GLU:HG3	2.19	0.42
1:A:286:LEU:HD12	1:A:315:ARG:CZ	2.50	0.42
1:A:178:GLU:OE1	1:A:178:GLU:N	2.44	0.42
1:A:180:ASN:C	1:A:180:ASN:ND2	2.71	0.42
1:A:5:VAL:HA	1:A:20:ARG:O	2.20	0.41
1:A:157:ARG:HG3	1:A:423:LEU:HD21	2.02	0.41
1:A:230:ARG:NH2	3:A:1001:SO4:O2	2.52	0.41
1:A:30:VAL:HG13	1:A:31:GLN:N	2.35	0.41
2:B:33:HIS:O	2:B:50:ILE:HA	2.21	0.41
1:A:306:ASP:C	1:A:306:ASP:OD1	2.59	0.41
1:A:176:GLU:HB2	1:A:177:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:VAL:HG21	1:A:429:VAL:CG2	2.47	0.41
1:A:67:SER:HA	1:A:74:GLU:C	2.41	0.41
1:A:386:LEU:HD22	1:A:390:GLN:CG	2.51	0.41
1:A:114:LEU:HD12	1:A:114:LEU:HA	1.93	0.41
2:B:5:VAL:HG22	2:B:6:ALA:N	2.37	0.40
1:A:129:LEU:HD23	1:A:129:LEU:O	2.21	0.40
1:A:66:LYS:HD2	1:A:66:LYS:HA	1.95	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	454/482 (94%)	424 (93%)	23 (5%)	7 (2%)	13	12
2	B	129/150 (86%)	119 (92%)	6 (5%)	4 (3%)	5	3
All	All	583/632 (92%)	543 (93%)	29 (5%)	11 (2%)	10	8

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	SER
2	B	-11	TRP
2	B	-8	PRO
2	B	53	ASN
2	B	67	SER
1	A	53	ASN
1	A	39	LYS
1	A	245	THR
1	A	247	ARG
1	A	276	LEU
1	A	274	ASN

### 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	387/426 (91%)	357 (92%)	30 (8%)	16	19
2	B	105/127 (83%)	101 (96%)	4 (4%)	40	54
All	All	492/553 (89%)	458 (93%)	34 (7%)	19	24

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LEU
1	A	114	LEU
1	A	119	ASP
1	A	140	LEU
1	A	145	LEU
1	A	149	LEU
1	A	156	LEU
1	A	168	ARG
1	A	178	GLU
1	A	180	ASN
1	A	190	ARG
1	A	195	LEU
1	A	207	LEU
1	A	212	LEU
1	A	219	LYS
1	A	241	ASP
1	A	252	GLU
1	A	270	ARG
1	A	283	GLU
1	A	307	GLU
1	A	322	LEU
1	A	324	VAL
1	A	335	ASN
1	A	373	GLU
1	A	382	LEU
1	A	386	LEU
1	A	399	LEU

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Mol	Chain	Res	Type
1	A	423	LEU
1	A	425	LEU
1	A	426	LEU
2	B	39	LYS
2	B	96	LEU
2	B	111	ARG
2	B	117	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	HIS
1	A	144	ASN
1	A	180	ASN
1	A	287	GLN
1	A	326	ASN
1	A	335	ASN
1	A	372	GLN
1	A	388	GLN
1	A	390	GLN
1	A	398	HIS
1	A	424	ASN
2	B	47	HIS
2	B	115	ASN

### 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

5 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	1001	-	4,4,4	0.07	0	6,6,6	0.18	0
3	SO4	A	1002	-	4,4,4	0.13	0	6,6,6	0.10	0
3	SO4	A	1005	-	4,4,4	0.22	0	6,6,6	0.06	0
3	SO4	B	1003	-	4,4,4	0.23	0	6,6,6	0.12	0
3	SO4	B	1004	-	4,4,4	0.11	0	6,6,6	0.09	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	1001	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1002	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1005	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1003	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1004	-	-	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	SO4	1	0

## 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	456/482 (94%)	0.77	52 (11%) <b>7</b> <b>10</b>	31, 54, 122, 163	0
2	B	131/150 (87%)	0.51	19 (14%) <b>3</b> <b>5</b>	31, 49, 99, 121	0
All	All	587/632 (92%)	0.71	71 (12%) <b>6</b> <b>9</b>	31, 52, 116, 163	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	276	LEU	14.7
1	A	275	ASP	11.8
1	A	245	THR	10.7
1	A	244	GLY	8.1
1	A	247	ARG	7.8
1	A	246	THR	7.3
1	A	272	GLU	7.1
1	A	277	VAL	6.8
1	A	67	SER	5.9
1	A	274	ASN	5.9
1	A	57	VAL	5.8
1	A	249	VAL	5.6
1	A	55	GLU	5.5
2	B	-9	SER	5.2
1	A	243	PRO	5.0
1	A	56	ASP	4.9
2	B	37	ARG	4.8
1	A	248	ASP	4.8
1	A	278	GLU	4.7
1	A	280	LEU	4.6
1	A	242	ILE	4.6
2	B	67	SER	4.5
1	A	273	THR	4.5
1	A	37	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	54	GLY	4.1
2	B	77	VAL	3.9
2	B	1	MET	3.9
1	A	279	ARG	3.7
1	A	82	HIS	3.7
2	B	118	MET	3.6
1	A	52	GLU	3.6
1	A	86	LEU	3.5
2	B	54	GLY	3.4
2	B	-10	GLY	3.4
1	A	21	LEU	3.4
2	B	21	LEU	3.3
2	B	-8	PRO	3.3
1	A	250	ILE	3.3
1	A	53	ASN	3.2
1	A	35	ARG	3.2
2	B	-11	TRP	3.2
1	A	318	ASN	3.0
2	B	95	PHE	3.0
1	A	341	ASN	2.9
1	A	38	SER	2.9
1	A	51	HIS	2.9
1	A	-5	SER	2.9
2	B	53	ASN	2.8
1	A	408	GLU	2.8
2	B	19	LEU	2.8
1	A	1	MET	2.7
1	A	0	LEU	2.7
1	A	77	VAL	2.6
2	B	62	VAL	2.5
1	A	19	LEU	2.5
1	A	212	LEU	2.5
1	A	-3	VAL	2.5
2	B	69	LYS	2.5
1	A	39	LYS	2.4
1	A	97	LYS	2.4
1	A	294	ILE	2.3
1	A	304	PRO	2.3
1	A	347	ARG	2.2
1	A	49	TRP	2.2
1	A	241	ASP	2.2
1	A	33	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	39	LYS	2.2
2	B	55	GLU	2.1
2	B	79	VAL	2.1
1	A	13	LYS	2.0
1	A	297	PHE	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(Å <sup>2</sup> )	Q<0.9
3	SO4	A	1005	5/5	0.87	0.21	2.17	106,106,107,107	0
3	SO4	B	1003	5/5	0.85	0.16	0.29	116,117,118,118	0
3	SO4	B	1004	5/5	0.98	0.12	-0.19	69,70,71,72	0
3	SO4	A	1001	5/5	0.99	0.13	-0.23	37,40,42,43	0
3	SO4	A	1002	5/5	0.98	0.13	-0.42	66,67,67,68	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.