



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:46 PM GMT

PDB ID : 1Q7M  
Title : Cobalamin-dependent methionine synthase (MethH) from *Thermotoga maritima* (Oxidized, Monoclinic)  
Authors : Evans, J.C.; Huddler, D.P.; Hilgers, M.T.; Romanchuk, G.; Matthews, R.G.; Ludwig, M.L.  
Deposited on : 2003-08-19  
Resolution : 2.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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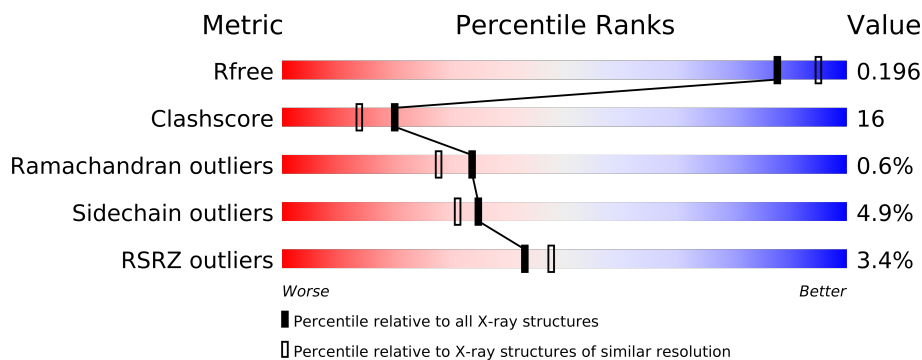
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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. 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	566	
1	B	566	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8962 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 5-methyltetrahydrofolateS-homocysteine methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	559	Total	C	N	O	S	0	0	0
			4423	2839	738	833	13			
1	B	548	Total	C	N	O	S	0	0	0
			4334	2782	724	815	13			

- Molecule 2 is water.

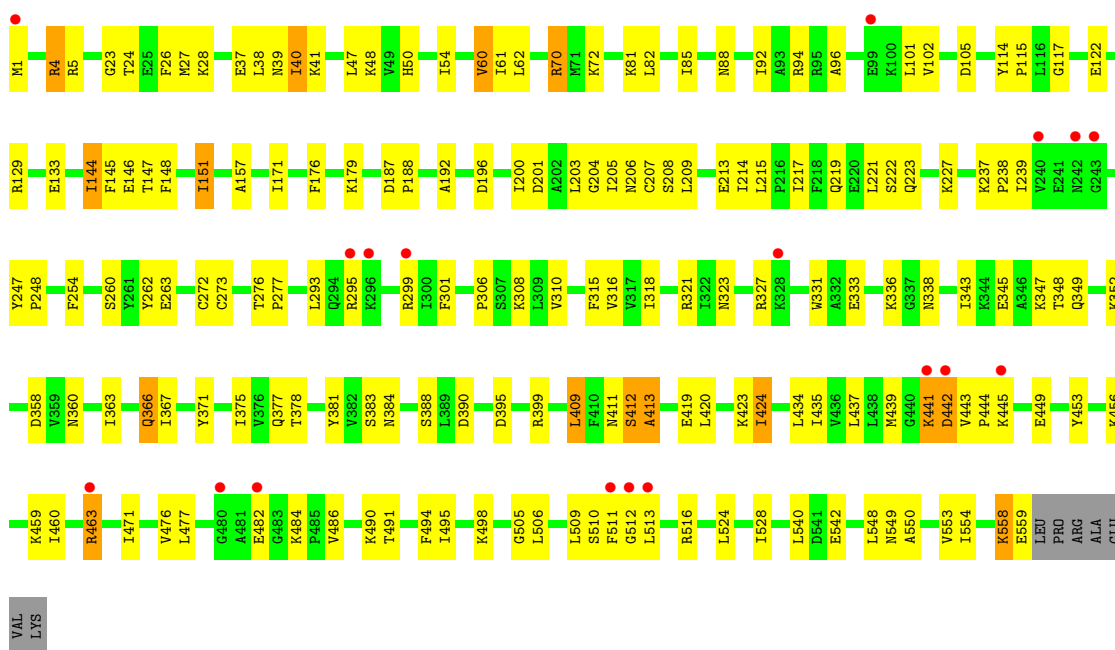
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	118	Total	O	0	0
			118	118		
2	B	87	Total	O	0	0
			87	87		

### 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.

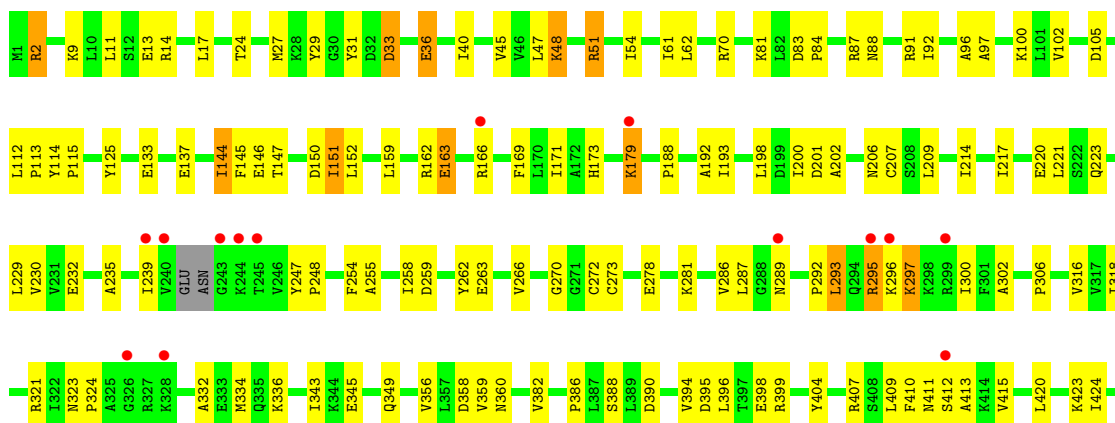
- Molecule 1: 5-methyltetrahydrofolateS-homocysteine methyltransferase

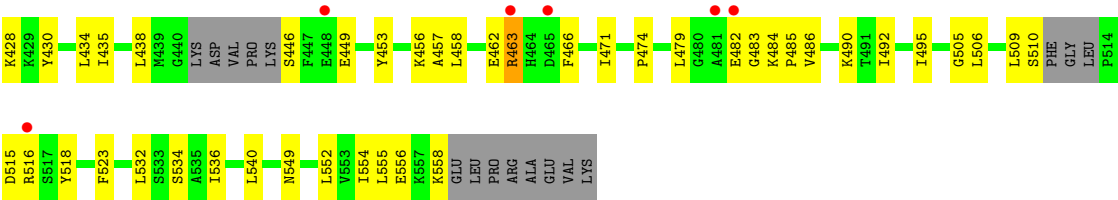
Chain A: 



- Molecule 1: 5-methyltetrahydrofolateS-homocysteine methyltransferase

Chain B: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.70Å 84.48Å 125.67Å 90.00° 100.87° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 18.75 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.10) 82.4 (18.75-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.66 (at 2.11Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.198 , 0.242 0.203 , 0.196	Depositor DCC
$R_{free}$ test set	5863 reflections (9.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.0	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 43.3	EDS
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.73$ , $\langle L^2 \rangle = 0.63$	Xtriage
Outliers	2 of 58895 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8962	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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	0.35	0/4505	0.63	2/6083 (0.0%)
1	B	0.32	0/4411	0.61	0/5951
All	All	0.34	0/8916	0.62	2/12034 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	413	ALA	N-CA-C	-5.35	96.55	111.00
1	A	505	GLY	N-CA-C	-5.11	100.33	113.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4423	0	4511	145	0
1	B	4334	0	4422	138	0
2	A	118	0	0	3	0
2	B	87	0	0	3	0
All	All	8962	0	8933	283	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 16.

All (283) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:29:TYR:OH	1:B:48:LYS:HG2	1.76	0.85
1:A:420:LEU:O	1:A:424:ILE:HD13	1.78	0.83
1:B:193:ILE:HD13	1:B:300:ILE:HD11	1.61	0.79
1:B:61:ILE:HD11	1:B:102:VAL:HG22	1.67	0.77
1:B:395:ASP:O	1:B:399:ARG:HD3	1.86	0.76
1:B:343:ILE:HD12	1:B:382:VAL:HG21	1.69	0.75
1:B:192:ALA:HB2	1:B:221:LEU:HD12	1.68	0.74
1:A:260:SER:O	1:A:263:GLU:HG2	1.86	0.74
1:B:48:LYS:NZ	1:B:48:LYS:HB2	2.03	0.73
1:A:524:LEU:O	1:A:528:ILE:HD13	1.88	0.73
1:B:144:ILE:HD12	1:B:146:GLU:HG2	1.70	0.72
1:A:144:ILE:HD12	1:A:146:GLU:HG2	1.71	0.72
1:B:413:ALA:HB2	1:B:434:LEU:HD11	1.72	0.72
1:A:491:THR:O	1:A:495:ILE:HD13	1.90	0.71
1:A:371:TYR:O	1:A:375:ILE:HD13	1.91	0.71
1:A:459:LYS:NZ	1:A:463:ARG:HH12	1.89	0.70
1:A:94:ARG:HD2	2:A:578:HOH:O	1.90	0.70
1:B:458:LEU:O	1:B:462:GLU:HG3	1.92	0.69
1:A:176:PHE:CE1	1:A:205:ILE:HD12	2.28	0.69
1:A:331:TRP:CH2	1:A:367:ILE:HD11	2.28	0.68
1:A:151:ILE:HD11	1:A:306:PRO:HG3	1.75	0.68
1:A:412:SER:H	1:A:435:ILE:HB	1.59	0.68
1:B:255:ALA:O	1:B:258:ILE:HD13	1.95	0.67
1:B:332:ALA:O	1:B:336:LYS:HG3	1.95	0.67
1:B:11:LEU:O	1:B:292:PRO:HG2	1.95	0.67
1:A:510:SER:OG	1:A:516:ARG:HB2	1.95	0.66
1:A:456:LYS:O	1:A:460:ILE:HD13	1.94	0.66
1:A:61:ILE:HD11	1:A:102:VAL:HG22	1.76	0.66
1:B:505:GLY:O	2:B:592:HOH:O	2.14	0.65
1:A:444:PRO:HG3	1:A:453:TYR:CE1	2.32	0.64
1:A:176:PHE:HE1	1:A:205:ILE:HD12	1.62	0.64
1:A:549:ASN:O	1:A:553:VAL:HG23	1.97	0.64
1:A:445:LYS:HG2	1:A:449:GLU:OE2	1.98	0.63
1:B:31:TYR:CE2	1:B:45:VAL:HG21	2.34	0.63
1:B:151:ILE:HD12	2:B:575:HOH:O	1.97	0.63
1:A:151:ILE:H	1:A:151:ILE:HD13	1.64	0.63
1:A:443:VAL:HG11	1:A:477:LEU:HD21	1.80	0.63
1:B:278:GLU:HA	1:B:281:LYS:HD2	1.81	0.63
1:B:510:SER:OG	1:B:516:ARG:HB2	2.00	0.62
1:A:437:LEU:HG	1:A:439:MET:HG2	1.82	0.62
1:B:390:ASP:HA	1:B:411:ASN:HB3	1.80	0.62
1:B:484:LYS:N	1:B:485:PRO:HD3	2.14	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:262:TYR:CZ	1:B:293:LEU:HD13	2.35	0.62
1:A:4:ARG:HD3	1:A:201:ASP:OD2	2.00	0.62
1:B:151:ILE:HD11	1:B:306:PRO:HG3	1.83	0.61
1:B:552:LEU:HD12	1:B:558:LYS:HZ1	1.65	0.61
1:A:390:ASP:HA	1:A:411:ASN:HB3	1.82	0.60
1:B:47:LEU:O	1:B:51:ARG:HD3	2.00	0.60
1:B:144:ILE:HG12	1:B:171:ILE:HB	1.84	0.60
1:B:144:ILE:HD13	1:B:145:PHE:N	2.17	0.59
1:A:413:ALA:HB2	1:A:434:LEU:HD11	1.84	0.59
1:B:438:LEU:HD11	1:B:495:ILE:HD11	1.83	0.59
1:A:206:ASN:ND2	1:A:207:CYS:SG	2.75	0.59
1:A:200:ILE:HD11	1:A:203:LEU:HD21	1.84	0.59
1:B:259:ASP:O	1:B:263:GLU:HG2	2.02	0.59
1:B:54:ILE:HD13	1:B:96:ALA:O	2.03	0.59
1:A:40:ILE:HG12	1:A:85:ILE:HD13	1.84	0.59
1:B:395:ASP:HB2	1:B:399:ARG:NH2	2.18	0.59
1:A:144:ILE:HD13	1:A:145:PHE:N	2.18	0.59
1:B:151:ILE:CD1	1:B:151:ILE:H	2.16	0.58
1:A:323:ASN:O	1:A:327:ARG:HD3	2.03	0.58
1:A:321:ARG:NE	1:A:540:LEU:HD22	2.18	0.58
1:A:367:ILE:HD12	1:A:367:ILE:N	2.18	0.58
1:A:204:GLY:O	1:A:205:ILE:HD13	2.03	0.58
1:A:205:ILE:HG21	1:A:214:ILE:HD12	1.85	0.58
1:A:40:ILE:HD12	1:A:88:ASN:ND2	2.18	0.58
1:B:318:ILE:CD1	1:B:356:VAL:HB	2.33	0.58
1:B:151:ILE:H	1:B:151:ILE:HD13	1.68	0.57
1:B:420:LEU:O	1:B:424:ILE:HG12	2.04	0.57
1:A:333:GLU:OE1	1:A:336:LYS:HD2	2.04	0.57
1:B:61:ILE:HD12	1:B:61:ILE:O	2.05	0.57
1:B:36:GLU:H	1:B:36:GLU:CD	2.07	0.57
1:A:144:ILE:C	1:A:144:ILE:HD13	2.25	0.57
1:A:459:LYS:HZ3	1:A:463:ARG:HH12	1.50	0.57
1:A:188:PRO:HG3	1:A:217:ILE:HG23	1.87	0.57
1:B:415:VAL:HG12	1:B:456:LYS:HE3	1.87	0.57
1:A:363:ILE:N	1:A:363:ILE:HD12	2.20	0.56
1:B:151:ILE:N	1:B:151:ILE:HD13	2.21	0.56
1:B:438:LEU:HD12	1:B:474:PRO:HA	1.86	0.56
1:A:321:ARG:CD	1:A:540:LEU:HD22	2.35	0.56
1:A:144:ILE:HD12	1:A:146:GLU:CG	2.35	0.56
1:B:255:ALA:HA	1:B:258:ILE:HD13	1.86	0.56
1:A:371:TYR:CE2	1:A:375:ILE:HD11	2.40	0.56
1:B:296:LYS:O	1:B:297:LYS:HB3	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:144:ILE:HD12	1:B:146:GLU:CG	2.35	0.56
1:A:363:ILE:H	1:A:363:ILE:HD12	1.70	0.56
1:A:81:LYS:O	1:A:85:ILE:HG12	2.06	0.56
1:B:321:ARG:NE	1:B:540:LEU:HD22	2.21	0.56
1:A:345:GLU:O	1:A:349:GLN:HG3	2.05	0.56
1:B:446:SER:HB3	1:B:449:GLU:HG3	1.88	0.56
1:B:193:ILE:CD1	1:B:300:ILE:HD11	2.35	0.55
1:A:214:ILE:HD11	2:A:589:HOH:O	2.06	0.55
1:A:151:ILE:HD13	1:A:151:ILE:N	2.21	0.55
1:B:100:LYS:HE2	2:B:626:HOH:O	2.06	0.55
1:A:315:PHE:CE1	1:A:528:ILE:HD11	2.41	0.55
1:A:151:ILE:H	1:A:151:ILE:CD1	2.20	0.55
1:B:318:ILE:HB	1:B:536:ILE:HA	1.89	0.55
1:A:196:ASP:O	1:A:227:LYS:HE3	2.06	0.55
1:A:40:ILE:HD12	1:A:88:ASN:HD22	1.72	0.55
1:A:115:PRO:HD3	1:A:378:THR:HA	1.88	0.55
1:A:476:VAL:HG11	1:A:509:LEU:HB2	1.88	0.55
1:A:441:LYS:O	1:A:442:ASP:CB	2.54	0.54
1:B:424:ILE:HD12	1:B:466:PHE:CD1	2.42	0.54
1:B:125:TYR:OH	1:B:163:GLU:HG2	2.07	0.54
1:A:441:LYS:O	1:A:442:ASP:HB2	2.08	0.54
1:A:61:ILE:HD12	1:A:61:ILE:O	2.07	0.54
1:A:409:LEU:CD2	1:A:435:ILE:HG13	2.38	0.53
1:B:9:LYS:HE2	1:B:13:GLU:OE2	2.08	0.53
1:A:331:TRP:CZ3	1:A:367:ILE:HD11	2.44	0.53
1:A:188:PRO:CG	1:A:217:ILE:HG23	2.39	0.53
1:A:366:GLN:C	1:A:367:ILE:HD12	2.29	0.53
1:B:97:ALA:O	1:B:100:LYS:HB2	2.09	0.52
1:A:50:HIS:O	1:A:54:ILE:HD12	2.09	0.52
1:B:133:GLU:O	1:B:137:GLU:HG3	2.10	0.52
1:B:318:ILE:HD12	1:B:356:VAL:HB	1.91	0.51
1:B:295:ARG:HG2	1:B:296:LYS:N	2.25	0.51
1:A:550:ALA:O	1:A:554:ILE:HG13	2.10	0.51
1:B:300:ILE:HD12	1:B:300:ILE:O	2.10	0.51
1:A:331:TRP:HH2	1:A:367:ILE:HD11	1.73	0.51
1:B:188:PRO:CG	1:B:217:ILE:HG23	2.40	0.51
1:A:60:VAL:HB	1:A:101:LEU:HB2	1.92	0.51
1:A:151:ILE:HD11	1:A:306:PRO:CG	2.40	0.51
1:B:474:PRO:HG3	1:B:492:ILE:HD11	1.92	0.51
1:A:558:LYS:HD3	1:A:559:GLU:O	2.10	0.51
1:B:235:ALA:O	1:B:247:TYR:HB3	2.10	0.51
1:A:333:GLU:HA	1:A:336:LYS:HG2	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:324:PRO:HG3	1:B:334:MET:SD	2.51	0.50
1:A:513:LEU:N	1:A:513:LEU:HD23	2.26	0.50
1:A:200:ILE:CD1	1:A:203:LEU:HD21	2.42	0.50
1:A:192:ALA:HB2	1:A:221:LEU:HD12	1.93	0.49
1:B:300:ILE:HD12	1:B:300:ILE:C	2.32	0.49
1:A:295:ARG:NH2	1:A:295:ARG:HB2	2.27	0.49
1:B:114:TYR:CD1	1:B:115:PRO:HA	2.48	0.48
1:A:129:ARG:O	1:A:133:GLU:HG3	2.13	0.48
1:B:302:ALA:O	1:B:407:ARG:HD3	2.12	0.48
1:B:144:ILE:HD13	1:B:144:ILE:C	2.34	0.48
1:A:61:ILE:C	1:A:61:ILE:HD12	2.34	0.48
1:B:152:LEU:HD13	1:B:152:LEU:C	2.34	0.48
1:A:348:THR:O	1:A:352:LYS:HD3	2.14	0.48
1:B:24:THR:HG22	1:B:27:MET:HE3	1.94	0.48
1:A:486:VAL:HG12	1:A:490:LYS:HE3	1.96	0.48
1:A:114:TYR:HA	1:A:117:GLY:O	2.14	0.48
1:B:47:LEU:HG	1:B:51:ARG:NE	2.29	0.48
1:A:321:ARG:HB2	1:A:349:GLN:CD	2.34	0.48
1:A:358:ASP:HA	1:A:388:SER:HB3	1.96	0.48
1:B:321:ARG:CD	1:B:540:LEU:HD22	2.44	0.48
1:B:200:ILE:C	1:B:200:ILE:HD12	2.33	0.48
1:B:81:LYS:C	1:B:84:PRO:HD2	2.33	0.48
1:B:358:ASP:HA	1:B:388:SER:HB3	1.96	0.48
1:B:424:ILE:O	1:B:428:LYS:HG3	2.13	0.47
1:B:435:ILE:HG12	1:B:471:ILE:CG2	2.45	0.47
1:B:316:VAL:O	1:B:534:SER:HB2	2.13	0.47
1:B:209:LEU:HD12	1:B:214:ILE:HD13	1.95	0.47
1:A:360:ASN:HB2	1:A:390:ASP:HB3	1.97	0.47
1:B:296:LYS:HB3	1:B:297:LYS:H	1.51	0.47
1:A:37:GLU:OE1	1:A:41:LYS:HE2	2.13	0.47
1:B:479:LEU:HD22	1:B:509:LEU:O	2.13	0.47
1:A:395:ASP:O	1:A:399:ARG:HD2	2.15	0.47
1:B:47:LEU:HD12	1:B:96:ALA:HB2	1.97	0.47
1:B:360:ASN:HB2	1:B:390:ASP:HB3	1.96	0.46
1:B:62:LEU:HB3	1:B:105:ASP:HB2	1.97	0.46
1:B:255:ALA:HB1	1:B:286:VAL:HG21	1.98	0.46
1:B:14:ARG:HA	1:B:292:PRO:HD3	1.96	0.46
1:A:549:ASN:OD1	1:A:558:LYS:HD2	2.14	0.46
1:A:333:GLU:HB3	1:A:338:ASN:HB3	1.97	0.46
1:A:445:LYS:HB2	1:A:484:LYS:NZ	2.31	0.46
1:B:61:ILE:HD12	1:B:61:ILE:C	2.36	0.46
1:A:129:ARG:NH1	1:A:133:GLU:OE2	2.49	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:70:ARG:HG3	1:B:70:ARG:HH21	1.80	0.46
1:A:40:ILE:N	1:A:40:ILE:HD13	2.31	0.46
1:B:229:LEU:HG	1:B:295:ARG:HH12	1.80	0.46
1:A:70:ARG:HH11	1:A:70:ARG:HB3	1.79	0.46
1:A:238:PRO:HB3	1:A:247:TYR:CE1	2.51	0.46
1:B:151:ILE:CD1	1:B:151:ILE:N	2.79	0.46
1:B:179:LYS:HE3	1:B:179:LYS:HA	1.97	0.46
1:A:419:GLU:OE1	1:A:423:LYS:NZ	2.46	0.46
1:B:410:PHE:HE2	1:B:423:LYS:HD3	1.80	0.45
1:B:9:LYS:O	1:B:13:GLU:HG3	2.16	0.45
1:A:219:GLN:O	1:A:223:GLN:HG3	2.16	0.45
1:B:318:ILE:HD13	1:B:356:VAL:HB	1.98	0.45
1:B:415:VAL:HG22	1:B:457:ALA:HB2	1.99	0.45
1:B:87:ARG:O	1:B:91:ARG:HG3	2.16	0.45
1:A:144:ILE:O	1:A:144:ILE:HG23	2.17	0.45
1:A:459:LYS:HZ1	1:A:463:ARG:HH12	1.65	0.45
1:B:263:GLU:OE2	1:B:263:GLU:HA	2.17	0.45
1:B:255:ALA:C	1:B:258:ILE:HD13	2.36	0.45
1:A:318:ILE:HD12	1:A:318:ILE:N	2.32	0.45
1:A:343:ILE:CG2	1:A:347:LYS:HZ3	2.29	0.45
1:A:262:TYR:CZ	1:A:293:LEU:HD13	2.52	0.45
1:B:262:TYR:HA	1:B:266:VAL:HG12	1.99	0.45
1:A:82:LEU:C	1:A:82:LEU:HD13	2.38	0.45
1:B:151:ILE:HD11	1:B:306:PRO:CG	2.47	0.44
1:A:509:LEU:O	1:A:509:LEU:HD22	2.18	0.44
1:A:409:LEU:HD21	1:A:435:ILE:HG13	1.97	0.44
1:A:445:LYS:O	1:A:484:LYS:HD2	2.17	0.44
1:A:145:PHE:HB3	1:A:148:PHE:CE1	2.52	0.44
1:B:188:PRO:HG2	1:B:217:ILE:HG23	1.98	0.44
1:A:409:LEU:HD22	1:A:435:ILE:HG13	2.00	0.44
1:A:144:ILE:HD12	1:A:146:GLU:CD	2.37	0.44
1:B:549:ASN:OD1	1:B:558:LYS:NZ	2.42	0.44
1:B:515:ASP:HB3	1:B:518:TYR:HD1	1.83	0.44
1:A:144:ILE:C	1:A:144:ILE:CD1	2.86	0.44
1:A:222:SER:HB2	1:A:295:ARG:CD	2.48	0.43
1:A:24:THR:O	1:A:28:LYS:HG3	2.18	0.43
1:A:26:PHE:CD1	1:A:38:LEU:HD12	2.52	0.43
1:A:327:ARG:HG2	1:A:327:ARG:HH11	1.83	0.43
1:B:394:VAL:HG13	1:B:395:ASP:N	2.33	0.43
1:A:222:SER:O	1:A:295:ARG:HD2	2.17	0.43
1:B:144:ILE:HG23	1:B:144:ILE:O	2.18	0.43
1:B:474:PRO:HG3	1:B:492:ILE:CD1	2.49	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:48:LYS:HZ2	1:B:48:LYS:HB2	1.80	0.43
1:B:24:THR:HA	1:B:27:MET:CE	2.48	0.43
1:B:33:ASP:N	1:B:33:ASP:OD1	2.48	0.43
1:B:386:PRO:HA	1:B:404:TYR:OH	2.19	0.43
1:A:377:GLN:O	1:A:381:TYR:HD1	2.01	0.43
1:B:144:ILE:HD12	1:B:146:GLU:CD	2.39	0.43
1:B:413:ALA:CB	1:B:434:LEU:HD11	2.45	0.43
1:A:207:CYS:O	1:A:208:SER:HB2	2.19	0.43
1:A:213:GLU:OE2	1:A:237:LYS:HG2	2.19	0.43
1:B:173:HIS:NE2	1:B:230:VAL:HB	2.33	0.43
1:B:232:GLU:HA	1:B:270:GLY:O	2.19	0.43
1:B:171:ILE:HG12	1:B:202:ALA:HB3	2.00	0.43
1:B:463:ARG:HH21	1:B:463:ARG:HG3	1.83	0.43
1:B:486:VAL:O	1:B:490:LYS:HG3	2.17	0.43
1:A:62:LEU:HB3	1:A:105:ASP:HB2	2.01	0.43
1:B:188:PRO:HG3	1:B:217:ILE:HG23	2.00	0.43
1:A:383:SER:O	1:A:384:ASN:HB2	2.19	0.42
1:B:272:CYS:SG	1:B:273:CYS:N	2.91	0.42
1:A:510:SER:HA	1:A:513:LEU:HD21	2.01	0.42
1:A:88:ASN:O	1:A:92:ILE:HG13	2.20	0.42
1:B:297:LYS:O	1:B:297:LYS:HG3	2.19	0.42
1:B:409:LEU:HD11	1:B:435:ILE:HG13	2.01	0.42
1:B:482:GLU:HA	1:B:482:GLU:OE1	2.18	0.42
1:B:113:PRO:HG2	1:B:150:ASP:OD2	2.18	0.42
1:A:176:PHE:HE1	1:A:205:ILE:CD1	2.30	0.42
1:B:492:ILE:HD12	1:B:532:LEU:HD13	2.02	0.42
1:B:2:ARG:HB2	1:B:2:ARG:HE	1.63	0.42
1:A:39:ASN:C	1:A:40:ILE:HD13	2.40	0.42
1:B:206:ASN:ND2	1:B:207:CYS:SG	2.93	0.42
1:A:276:THR:HB	1:A:277:PRO:HD2	2.01	0.42
1:A:151:ILE:HD12	2:A:635:HOH:O	2.19	0.42
1:A:316:VAL:O	1:A:318:ILE:HD12	2.19	0.42
1:A:23:GLY:O	1:A:27:MET:HG3	2.19	0.42
1:B:162:ARG:HD2	1:B:166:ARG:HA	2.01	0.42
1:A:145:PHE:CE2	1:A:157:ALA:HB1	2.54	0.42
1:B:509:LEU:CD2	1:B:523:PHE:HB2	2.50	0.41
1:A:363:ILE:O	1:A:367:ILE:CD1	2.68	0.41
1:A:301:PHE:CZ	1:A:471:ILE:HG13	2.55	0.41
1:A:215:LEU:HD13	1:A:215:LEU:C	2.40	0.41
1:A:276:THR:HB	1:A:277:PRO:CD	2.50	0.41
1:B:14:ARG:NH2	1:B:289:ASN:OD1	2.54	0.41
1:B:321:ARG:O	1:B:323:ASN:N	2.52	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:144:ILE:HG12	1:A:171:ILE:HB	2.02	0.41
1:B:345:GLU:O	1:B:349:GLN:HG3	2.19	0.41
1:A:1:MET:SD	1:A:94:ARG:NH2	2.93	0.41
1:A:239:ILE:HD13	1:A:248:PRO:HG3	2.03	0.41
1:A:48:LYS:HE3	1:A:48:LYS:HB2	1.88	0.41
1:B:398:GLU:HG3	1:B:430:TYR:CE2	2.55	0.41
1:B:17:LEU:HD13	1:B:287:LEU:HD22	2.03	0.41
1:A:308:LYS:HE3	1:A:310:VAL:CG2	2.51	0.41
1:A:443:VAL:HG11	1:A:477:LEU:CD2	2.49	0.41
1:B:162:ARG:CD	1:B:166:ARG:HA	2.51	0.41
1:B:554:ILE:C	1:B:556:GLU:H	2.23	0.41
1:A:5:ARG:HG3	1:A:5:ARG:HH21	1.86	0.41
1:B:151:ILE:HD11	1:B:306:PRO:CB	2.51	0.41
1:A:54:ILE:HD13	1:A:96:ALA:O	2.21	0.41
1:B:247:TYR:HA	1:B:248:PRO:HD2	1.95	0.41
1:A:494:PHE:O	1:A:498:LYS:HG2	2.21	0.41
1:B:359:VAL:HG23	1:B:359:VAL:O	2.21	0.41
1:B:169:PHE:CE1	1:B:201:ASP:HB3	2.56	0.41
1:A:272:CYS:SG	1:A:273:CYS:N	2.94	0.41
1:A:40:ILE:HG12	1:A:85:ILE:CD1	2.49	0.40
1:A:321:ARG:HH11	1:A:321:ARG:HG2	1.87	0.40
1:A:187:ASP:C	1:A:187:ASP:OD2	2.59	0.40
1:B:88:ASN:O	1:B:92:ILE:HG13	2.21	0.40
1:A:412:SER:HA	1:A:435:ILE:O	2.21	0.40
1:A:247:TYR:HA	1:A:248:PRO:HD2	1.93	0.40
1:A:47:LEU:HD12	1:A:96:ALA:HB2	2.04	0.40
1:B:255:ALA:HA	1:B:258:ILE:CD1	2.51	0.40
1:B:40:ILE:HD11	1:B:84:PRO:HB2	2.03	0.40
1:A:460:ILE:N	1:A:460:ILE:HD12	2.37	0.40
1:B:510:SER:CB	1:B:516:ARG:HB2	2.51	0.40
1:A:209:LEU:HB3	1:A:213:GLU:HB2	2.04	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	557/566 (98%)	529 (95%)	25 (4%)	3 (0%)	38	33
1	B	540/566 (95%)	518 (96%)	18 (3%)	4 (1%)	30	23
All	All	1097/1132 (97%)	1047 (95%)	43 (4%)	7 (1%)	33	28

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	412	SER
1	A	442	ASP
1	B	297	LYS
1	B	412	SER
1	A	512	GLY
1	B	506	LEU
1	B	483	GLY

### 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	488/494 (99%)	465 (95%)	23 (5%)	36	33
1	B	478/494 (97%)	454 (95%)	24 (5%)	34	30
All	All	966/988 (98%)	919 (95%)	47 (5%)	35	31

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	40	ILE
1	A	60	VAL
1	A	70	ARG
1	A	72	LYS
1	A	122	GLU
1	A	144	ILE
1	A	147	THR
1	A	151	ILE
1	A	179	LYS

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Mol	Chain	Res	Type
1	A	254	PHE
1	A	299	ARG
1	A	366	GLN
1	A	409	LEU
1	A	424	ILE
1	A	441	LYS
1	A	463	ARG
1	A	482	GLU
1	A	506	LEU
1	A	511	PHE
1	A	542	GLU
1	A	548	LEU
1	A	558	LYS
1	B	2	ARG
1	B	33	ASP
1	B	36	GLU
1	B	48	LYS
1	B	51	ARG
1	B	83	ASP
1	B	112	LEU
1	B	144	ILE
1	B	147	THR
1	B	151	ILE
1	B	159	LEU
1	B	163	GLU
1	B	179	LYS
1	B	198	LEU
1	B	220	GLU
1	B	223	GLN
1	B	239	ILE
1	B	254	PHE
1	B	293	LEU
1	B	295	ARG
1	B	396	LEU
1	B	453	TYR
1	B	463	ARG
1	B	555	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN

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Mol	Chain	Res	Type
1	A	393	ASN
1	B	501	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 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	559/566 (98%)	0.05	18 (3%)	45 50	16, 26, 47, 62	0
1	B	548/566 (96%)	0.13	20 (3%)	41 45	17, 32, 53, 67	0
All	All	1107/1132 (97%)	0.09	38 (3%)	43 47	16, 29, 51, 67	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	511	PHE	7.7
1	B	240	VAL	5.1
1	A	296	LYS	4.5
1	B	244	LYS	4.5
1	B	296	LYS	4.1
1	A	242	ASN	4.0
1	A	512	GLY	4.0
1	A	442	ASP	3.9
1	B	239	ILE	3.8
1	A	513	LEU	3.8
1	B	328	LYS	3.8
1	A	441	LYS	3.6
1	B	243	GLY	3.5
1	B	482	GLU	3.5
1	B	299	ARG	3.3
1	B	245	THR	3.2
1	B	289	ASN	3.2
1	A	243	GLY	3.2
1	B	448	GLU	3.2
1	A	299	ARG	3.1
1	B	481	ALA	3.1
1	A	240	VAL	3.1
1	A	480	GLY	3.1
1	A	445	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	328	LYS	3.0
1	B	326	GLY	2.9
1	B	465	ASP	2.9
1	A	99	GLU	2.9
1	B	295	ARG	2.8
1	A	1	MET	2.8
1	B	412	SER	2.7
1	B	179	LYS	2.5
1	B	166	ARG	2.5
1	A	295	ARG	2.3
1	B	463	ARG	2.2
1	A	463	ARG	2.1
1	A	482	GLU	2.0
1	B	516	ARG	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 ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.