



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:41 PM GMT

PDB ID : 1Q7M  
Title : Cobalamin-dependent methionine synthase (MetH) 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 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

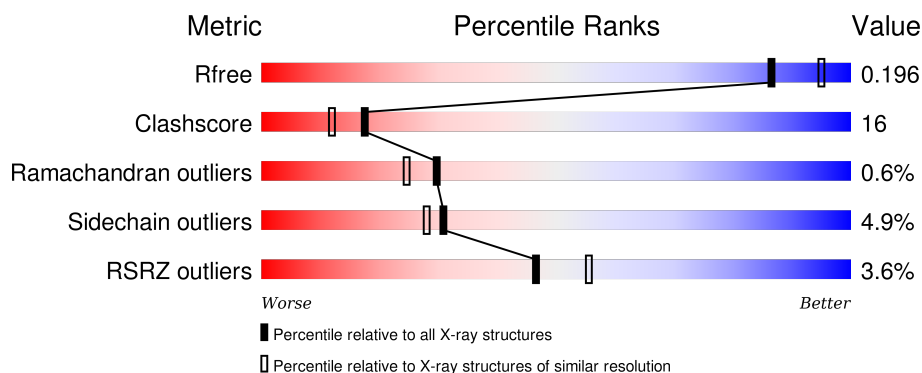
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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. 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	566	<div> <div>3%</div> <div>68%</div> <div>28%</div> <div>..</div> </div>
1	B	566	<div> <div>4%</div> <div>65%</div> <div>29%</div> <div>..</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8962 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 5-methyltetrahydrofolate S-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			

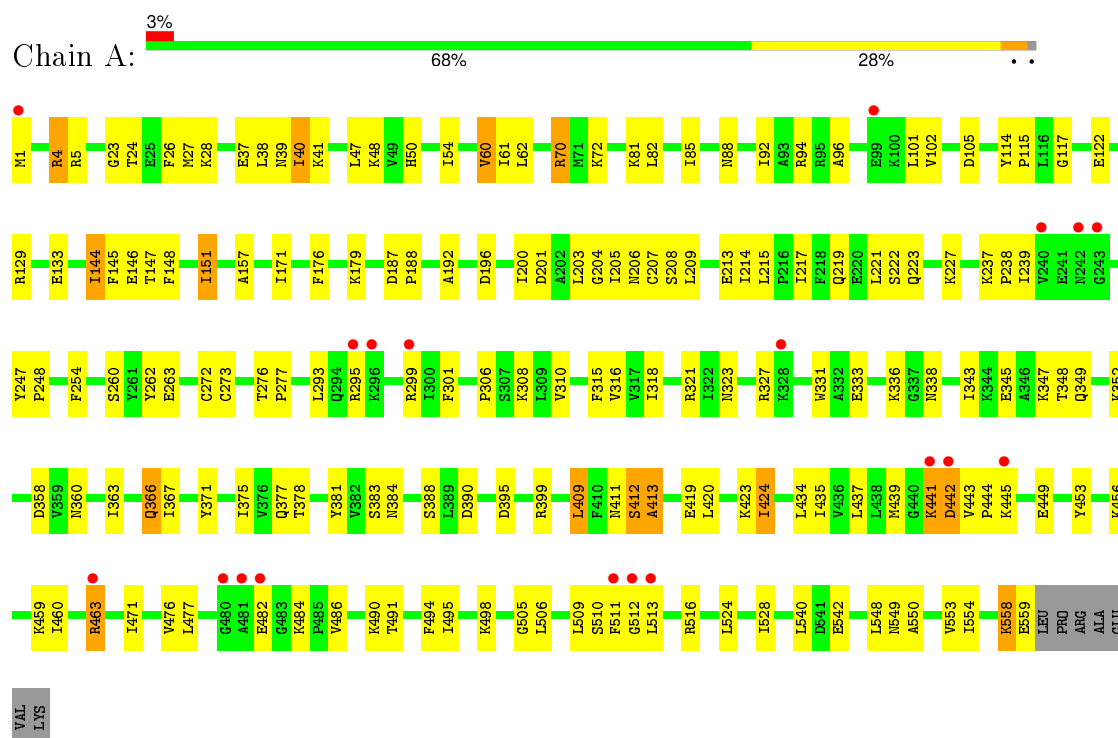
- Molecule 2 is water.

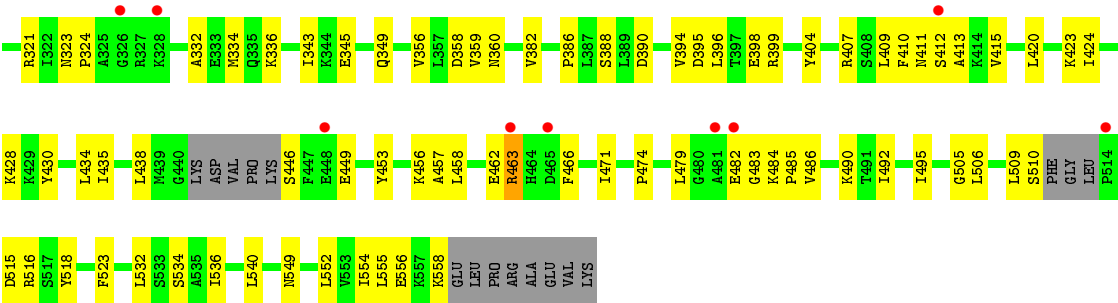
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	118	Total	O	0	0
			118	118		
2	B	87	Total	O	0	0
			87	87		

### 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-methyltetrahydrofolate S-homocysteine methyltransferase





## 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 , 52.5	EDS
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.73$ , $\langle L^2 \rangle = 0.63$	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.

<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 [i](#)

### 5.1 Standard geometry [i](#)

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 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	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

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 (283) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:LYS:N	1:B:485:PRO:HD3	2.14	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 [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	557/566 (98%)	529 (95%)	25 (4%)	3 (0%)	34	30
1	B	540/566 (95%)	518 (96%)	18 (3%)	4 (1%)	26	21
All	All	1097/1132 (97%)	1047 (95%)	43 (4%)	7 (1%)	30	24

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 [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	488/494 (99%)	465 (95%)	23 (5%)	32	30
1	B	478/494 (97%)	454 (95%)	24 (5%)	30	27
All	All	966/988 (98%)	919 (95%)	47 (5%)	31	28

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
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

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

### 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](#)

There are no ligands in this entry.

## 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	559/566 (98%)	0.04	19 (3%)	49 58	16, 26, 47, 62	0
1	B	548/566 (96%)	0.13	21 (3%)	44 53	17, 32, 53, 67	0
All	All	1107/1132 (97%)	0.08	40 (3%)	46 55	16, 29, 51, 67	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	511	PHE	8.6
1	B	240	VAL	5.9
1	B	244	LYS	4.9
1	A	296	LYS	4.5
1	B	296	LYS	4.3
1	B	239	ILE	4.2
1	A	242	ASN	4.1
1	A	512	GLY	3.9
1	B	328	LYS	3.9
1	A	442	ASP	3.9
1	A	513	LEU	3.7
1	B	243	GLY	3.6
1	B	245	THR	3.6
1	B	482	GLU	3.5
1	A	240	VAL	3.3
1	B	326	GLY	3.3
1	B	481	ALA	3.3
1	B	299	ARG	3.2
1	A	328	LYS	3.2
1	A	299	ARG	3.2
1	B	412	SER	3.1
1	A	243	GLY	3.1
1	A	441	LYS	3.1
1	B	448	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	465	ASP	3.1
1	A	445	LYS	3.1
1	A	1	MET	3.0
1	A	99	GLU	2.9
1	B	289	ASN	2.9
1	A	480	GLY	2.9
1	B	179	LYS	2.8
1	B	295	ARG	2.8
1	B	166	ARG	2.5
1	B	266	VAL	2.4
1	A	463	ARG	2.4
1	B	463	ARG	2.3
1	A	482	GLU	2.2
1	A	295	ARG	2.2
1	A	481	ALA	2.1
1	B	514	PRO	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.