



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 4, 2024 – 07:07 AM EST

PDB ID : 1Q7Z  
Title : Cobalamin-dependent methionine synthase (1-566) from *Thermotoga maritima* (Cd<sup>2+</sup> complex)  
Authors : Evans, J.C.; Huddler, D.P.; Hilgers, M.T.; Romanchuk, G.; Matthews, R.G.; Ludwig, M.L.  
Deposited on : 2003-08-20  
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

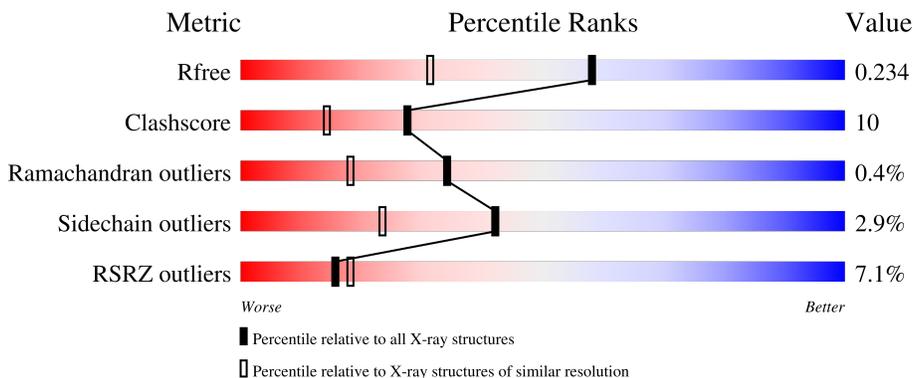
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	566	 7% 77% 20% ..
1	B	566	 7% 72% 23% ..

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9111 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
			Total	C	N	O	S			
1	A	559	4423	2839	738	833	13	0	0	0
1	B	548	4334	2782	724	815	13	0	0	0

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Cd 1	0	0
2	B	1	Total 1	Cd 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	198	Total 198	O 198	0	0
3	B	154	Total 154	O 154	0	0





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.54Å 85.13Å 125.61Å 90.00° 100.86° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 19.68 – 1.65	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.70) 95.9 (19.68-1.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 1.65Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.216 , 0.237 0.212 , 0.234	Depositor DCC
$R_{free}$ test set	6503 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtrriage
Anisotropy	0.296	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 56.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9111	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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: CD

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	0.32	0/4505	0.62	3/6083 (0.0%)
1	B	0.29	0/4411	0.58	0/5951
All	All	0.31	0/8916	0.60	3/12034 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	413	ALA	N-CA-C	-6.55	93.31	111.00
1	A	505	GLY	N-CA-C	-5.55	99.23	113.10
1	A	412	SER	N-CA-C	5.08	124.71	111.00

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	4510	91	0
1	B	4334	0	4421	88	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	198	0	0	2	0
3	B	154	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9111	0	8931	177	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 10.

All (177) 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:361:PHE:HB3	1:B:367:ILE:HD12	1.40	1.03
1:A:296:LYS:HG2	1:A:297:LYS:H	1.33	0.94
1:A:144:ILE:HD11	1:A:173:HIS:CE1	2.13	0.84
1:B:239:ILE:HD13	1:B:240:VAL:N	1.96	0.81
1:B:47:LEU:O	1:B:51:ARG:HD3	1.83	0.77
1:A:412:SER:H	1:A:435:ILE:HB	1.54	0.73
1:B:395:ASP:O	1:B:399:ARG:HD3	1.88	0.72
1:A:1:MET:HG2	1:A:139:GLY:O	1.90	0.72
1:A:115:PRO:HG3	1:A:378:THR:HG23	1.73	0.71
1:B:11:LEU:O	1:B:292:PRO:HG2	1.92	0.69
1:B:179:LYS:HE3	1:B:179:LYS:HA	1.75	0.67
1:A:486:VAL:HG12	1:A:490:LYS:HE3	1.75	0.67
1:B:515:ASP:HB3	1:B:518:TYR:HD1	1.59	0.66
1:B:70:ARG:HD2	1:B:130:GLU:OE1	1.95	0.66
1:A:558:LYS:HD3	1:A:559:GLU:N	2.11	0.66
1:A:443:VAL:HG11	1:A:477:LEU:HD21	1.79	0.65
1:A:412:SER:HA	1:A:435:ILE:O	1.95	0.65
1:B:70:ARG:HG2	1:B:79:GLU:OE2	1.97	0.65
1:A:510:SER:HA	1:A:513:LEU:HD21	1.79	0.64
1:B:144:ILE:HD11	1:B:173:HIS:CE1	2.32	0.64
1:A:200:ILE:HD11	1:A:203:LEU:HD21	1.79	0.64
1:A:5:ARG:HB3	1:A:5:ARG:NH2	2.12	0.64
1:A:296:LYS:HG2	1:A:297:LYS:N	2.10	0.62
1:A:390:ASP:HA	1:A:411:ASN:HB3	1.82	0.62
1:B:361:PHE:HB3	1:B:367:ILE:CD1	2.23	0.62
1:B:59:ASP:HA	1:B:100:LYS:HE3	1.82	0.61
1:B:324:PRO:HG3	1:B:334:MET:SD	2.39	0.61
1:B:479:LEU:HD22	1:B:509:LEU:O	2.00	0.60
1:B:193:ILE:HD11	1:B:300:ILE:HD11	1.83	0.60
1:A:476:VAL:HG11	1:A:509:LEU:HB2	1.84	0.60
1:B:193:ILE:CD1	1:B:300:ILE:HD11	2.32	0.59
1:A:223:GLN:HB3	1:A:298:LYS:HZ3	1.66	0.59
1:B:413:ALA:HB2	1:B:434:LEU:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HB2	1:A:141:ASP:OD1	2.03	0.59
1:B:479:LEU:HD23	1:B:480:GLY:H	1.68	0.58
1:B:31:TYR:CE2	1:B:45:VAL:HG21	2.38	0.58
1:B:296:LYS:O	1:B:297:LYS:HB3	2.02	0.58
1:A:241:GLU:O	1:A:244:LYS:HG2	2.04	0.58
1:A:3:ASN:OD1	1:A:5:ARG:HG2	2.04	0.57
1:B:347:LYS:O	1:B:351:GLU:HG3	2.04	0.57
1:B:484:LYS:N	1:B:485:PRO:HD3	2.19	0.57
1:B:188:PRO:HG3	1:B:217:ILE:HG23	1.87	0.57
1:B:200:ILE:CD1	1:B:203:LEU:HD21	2.35	0.57
1:B:188:PRO:CG	1:B:217:ILE:HG23	2.35	0.57
1:A:513:LEU:HD23	1:A:513:LEU:N	2.19	0.56
1:A:1:MET:HG3	1:A:94:ARG:NH2	2.20	0.56
1:B:510:SER:OG	1:B:516:ARG:HB2	2.05	0.56
1:B:536:ILE:N	1:B:536:ILE:HD12	2.21	0.56
1:A:393:ASN:OD1	1:A:395:ASP:HB3	2.06	0.56
1:A:510:SER:OG	1:A:516:ARG:HB2	2.05	0.56
1:A:463:ARG:HB3	1:A:463:ARG:HH21	1.71	0.55
1:B:358:ASP:HA	1:B:388:SER:HB3	1.89	0.55
1:B:332:ALA:O	1:B:336:LYS:HG3	2.07	0.55
1:B:458:LEU:O	1:B:462:GLU:HG3	2.07	0.55
1:A:37:GLU:OE1	1:A:41:LYS:HE2	2.06	0.54
1:A:308:LYS:HE3	1:A:310:VAL:HG22	1.89	0.54
1:B:446:SER:OG	1:B:449:GLU:HG3	2.07	0.54
1:B:516:ARG:HG3	1:B:517:SER:N	2.21	0.54
1:B:162:ARG:HD2	1:B:166:ARG:HA	1.90	0.54
1:A:463:ARG:HH21	1:A:463:ARG:CB	2.21	0.53
1:A:196:ASP:O	1:A:227:LYS:HE3	2.08	0.53
1:A:308:LYS:HE3	1:A:310:VAL:CG2	2.39	0.53
1:A:402:ARG:HG2	1:A:430:TYR:CE1	2.44	0.52
1:A:463:ARG:HD2	1:A:464:HIS:CE1	2.44	0.52
1:A:515:ASP:HB3	1:A:518:TYR:HD1	1.75	0.52
1:B:114:TYR:CD1	1:B:115:PRO:HA	2.45	0.52
1:A:463:ARG:HG3	1:A:464:HIS:ND1	2.25	0.51
1:B:47:LEU:HD12	1:B:96:ALA:HB2	1.93	0.51
1:B:192:ALA:HB2	1:B:221:LEU:HD12	1.92	0.51
1:A:444:PRO:HG3	1:A:453:TYR:CE1	2.45	0.51
1:B:188:PRO:HB2	1:B:220:GLU:HB3	1.93	0.51
1:B:200:ILE:HD11	1:B:203:LEU:HD21	1.92	0.51
1:A:321:ARG:HB2	1:A:349:GLN:NE2	2.25	0.51
1:A:188:PRO:CG	1:A:217:ILE:HG23	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:LYS:CG	1:A:297:LYS:H	2.15	0.51
1:A:219:GLN:O	1:A:223:GLN:HG3	2.10	0.51
1:A:333:GLU:HA	1:A:336:LYS:HG2	1.92	0.51
1:B:390:ASP:HA	1:B:411:ASN:HB3	1.91	0.51
1:A:115:PRO:HD3	1:A:378:THR:HA	1.92	0.50
1:B:262:TYR:CZ	1:B:293:LEU:HD13	2.46	0.50
1:A:301:PHE:CZ	1:A:471:ILE:HG13	2.47	0.50
1:B:321:ARG:HD2	1:B:540:LEU:HD13	1.94	0.50
1:A:299:ARG:HH11	1:A:299:ARG:HG3	1.77	0.50
1:A:395:ASP:O	1:A:399:ARG:HD3	2.11	0.50
1:B:536:ILE:HD12	1:B:536:ILE:H	1.77	0.50
1:A:200:ILE:CD1	1:A:203:LEU:HD21	2.39	0.49
1:B:321:ARG:NE	1:B:540:LEU:HD22	2.27	0.49
1:B:240:VAL:HA	1:B:244:LYS:O	2.12	0.49
1:A:437:LEU:HG	1:A:439:MET:HG2	1.93	0.49
1:B:125:TYR:CE1	1:B:160:ALA:HA	2.48	0.48
1:B:129:ARG:O	1:B:133:GLU:HG3	2.12	0.48
1:B:9:LYS:O	1:B:13:GLU:HG3	2.14	0.48
1:A:14:ARG:CZ	1:A:289:ASN:OD1	2.62	0.48
1:A:553:VAL:HG22	1:A:559:GLU:HA	1.96	0.48
1:A:5:ARG:HB3	1:A:5:ARG:HH21	1.76	0.47
1:B:47:LEU:HG	1:B:51:ARG:NE	2.29	0.47
1:A:486:VAL:CG1	1:A:490:LYS:HE3	2.43	0.47
1:A:358:ASP:HA	1:A:388:SER:HB3	1.97	0.47
1:A:383:SER:O	1:A:384:ASN:HB2	2.15	0.47
1:A:463:ARG:HB3	1:A:463:ARG:NH2	2.30	0.47
1:B:330:LEU:O	1:B:334:MET:HG3	2.14	0.47
1:A:252:HIS:O	1:A:256:VAL:HG13	2.15	0.47
1:A:9:LYS:O	1:A:13:GLU:HG3	2.15	0.47
1:A:192:ALA:HB2	1:A:221:LEU:HD12	1.95	0.47
1:A:193:ILE:CD1	1:A:300:ILE:HD11	2.45	0.46
1:A:209:LEU:HB3	1:A:213:GLU:HB2	1.96	0.46
1:B:259:ASP:O	1:B:263:GLU:HG2	2.16	0.46
1:A:209:LEU:HB2	1:A:214:ILE:HG13	1.97	0.46
1:A:509:LEU:O	1:A:509:LEU:HD13	2.15	0.46
1:B:209:LEU:HB2	1:B:214:ILE:HG13	1.97	0.46
1:B:412:SER:H	1:B:435:ILE:HB	1.81	0.46
1:B:162:ARG:HD3	1:B:162:ARG:HA	1.68	0.45
1:A:188:PRO:HG3	1:A:217:ILE:HG23	1.98	0.45
1:A:441:LYS:O	1:A:442:ASP:HB3	2.16	0.45
1:A:252:HIS:HB3	3:A:673:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:VAL:O	1:B:248:PRO:HD3	2.17	0.45
1:A:509:LEU:HD13	1:A:509:LEU:C	2.37	0.45
1:A:238:PRO:HB3	1:A:247:TYR:CE1	2.52	0.45
1:B:457:ALA:O	1:B:461:LEU:HG	2.17	0.45
1:A:347:LYS:O	1:A:351:GLU:HG3	2.17	0.45
1:B:35:PRO:HG2	1:B:36:GLU:OE2	2.17	0.45
1:A:129:ARG:NH1	1:A:133:GLU:OE2	2.50	0.45
1:A:330:LEU:O	1:A:334:MET:HG3	2.17	0.44
1:B:2:ARG:N	1:B:2:ARG:HD3	2.33	0.44
1:B:17:LEU:HD13	1:B:287:LEU:CD2	2.47	0.44
1:A:23:GLY:O	1:A:27:MET:HG3	2.18	0.44
1:B:238:PRO:HB2	1:B:245:THR:HG23	2.00	0.44
1:A:360:ASN:HB2	1:A:390:ASP:HB3	2.00	0.44
1:B:34:LEU:HB2	1:B:37:GLU:HG3	1.99	0.44
1:A:144:ILE:HD13	1:A:146:GLU:OE1	2.17	0.43
1:B:209:LEU:HB3	1:B:213:GLU:HB2	1.99	0.43
1:A:188:PRO:HG2	1:A:217:ILE:HG23	1.99	0.43
1:A:162:ARG:HD2	1:A:166:ARG:HG3	2.00	0.43
1:B:451:LYS:HE3	1:B:494:PHE:CZ	2.54	0.43
1:B:474:PRO:HD2	1:B:503:THR:O	2.18	0.43
1:A:67:GLY:HA2	1:A:72:LYS:HD3	1.99	0.43
1:B:364:GLU:HB3	1:B:396:LEU:HD12	2.00	0.43
1:B:152:LEU:CD2	1:B:377:GLN:HG3	2.49	0.43
1:B:44:ASP:HB2	3:B:682:HOH:O	2.19	0.43
1:B:398:GLU:HG3	1:B:430:TYR:CE2	2.53	0.43
1:A:129:ARG:O	1:A:133:GLU:HG3	2.18	0.43
1:B:383:SER:O	1:B:384:ASN:HB2	2.19	0.43
1:B:427:LEU:CD1	1:B:434:LEU:HB2	2.48	0.43
1:A:373:GLU:HB3	3:A:688:HOH:O	2.18	0.42
1:A:397:THR:HG23	1:A:410:PHE:CE1	2.53	0.42
1:B:24:THR:HA	1:B:27:MET:HE3	2.00	0.42
1:B:360:ASN:HB2	1:B:390:ASP:HB3	1.99	0.42
1:A:398:GLU:HG3	1:A:430:TYR:CE2	2.53	0.42
1:B:59:ASP:O	1:B:100:LYS:HG3	2.19	0.42
1:A:474:PRO:HD2	1:A:503:THR:O	2.20	0.42
1:B:14:ARG:HA	1:B:292:PRO:HD3	2.02	0.42
1:B:247:TYR:HA	1:B:248:PRO:HD2	1.88	0.42
1:A:129:ARG:HG2	1:A:129:ARG:HH11	1.84	0.42
1:A:249:LEU:HD11	1:A:253:ASP:HB3	2.02	0.41
1:B:479:LEU:HD22	1:B:510:SER:HA	2.02	0.41
1:A:446:SER:OG	1:A:449:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:GLU:HA	1:B:270:GLY:O	2.20	0.41
1:A:476:VAL:CG1	1:A:509:LEU:HB2	2.50	0.41
1:B:359:VAL:HG23	1:B:359:VAL:O	2.19	0.41
1:A:181:ARG:CZ	1:A:185:GLY:O	2.68	0.41
1:B:188:PRO:HG2	1:B:217:ILE:HG23	2.00	0.41
1:B:230:VAL:HG22	1:B:268:ILE:HB	2.02	0.41
1:A:554:ILE:HG23	1:B:485:PRO:HB2	2.02	0.41
1:A:162:ARG:HD3	1:A:162:ARG:HA	1.82	0.41
1:A:494:PHE:O	1:A:498:LYS:HG2	2.21	0.41
1:A:558:LYS:HE3	1:A:558:LYS:HB2	1.97	0.41
1:B:132:VAL:HG11	1:B:161:ALA:HA	2.01	0.41
1:B:323:ASN:HA	1:B:324:PRO:HD3	1.91	0.41
1:A:321:ARG:HB2	1:A:349:GLN:CD	2.41	0.41
1:B:247:TYR:HB2	1:B:274:GLY:HA3	2.02	0.41
1:B:200:ILE:HD12	1:B:203:LEU:CD2	2.52	0.40
1:A:546:LYS:HD3	1:B:518:TYR:CE1	2.55	0.40
1:B:152:LEU:HD22	1:B:377:GLN:HG3	2.03	0.40
1:A:14:ARG:NH1	1:A:289:ASN:OD1	2.54	0.40
1:A:223:GLN:HB3	1:A:298:LYS:NZ	2.35	0.40
1:B:277:PRO:O	1:B:281:LYS:HG3	2.21	0.40
1:B:145:PHE:CE2	1:B:157:ALA:HB1	2.56	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%)	535 (96%)	21 (4%)	1 (0%)	47 30
1	B	540/566 (95%)	518 (96%)	19 (4%)	3 (1%)	25 11
All	All	1097/1132 (97%)	1053 (96%)	40 (4%)	4 (0%)	34 18

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	412	SER
1	B	412	SER
1	B	297	LYS
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%)	479 (98%)	9 (2%)	59	43
1	B	478/494 (97%)	459 (96%)	19 (4%)	31	13
All	All	966/988 (98%)	938 (97%)	28 (3%)	42	23

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	147	THR
1	A	248	PRO
1	A	254	PHE
1	A	295	ARG
1	A	366	GLN
1	A	463	ARG
1	A	513	LEU
1	A	558	LYS
1	B	2	ARG
1	B	33	ASP
1	B	48	LYS
1	B	51	ARG
1	B	70	ARG
1	B	94	ARG
1	B	147	THR
1	B	159	LEU
1	B	163	GLU
1	B	179	LYS

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Mol	Chain	Res	Type
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	396	LEU
1	B	463	ARG
1	B	555	LEU

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

Mol	Chain	Res	Type
1	B	294	GLN
1	B	349	GLN
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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 [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%)	0.24	39 (6%) 16 18	13, 24, 44, 54	0
1	B	548/566 (96%)	0.44	40 (7%) 15 17	16, 29, 47, 58	0
All	All	1107/1132 (97%)	0.34	79 (7%) 16 18	13, 26, 46, 58	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	511	PHE	11.4
1	B	244	LYS	7.6
1	B	296	LYS	6.1
1	B	240	VAL	5.9
1	A	442	ASP	5.6
1	A	512	GLY	5.5
1	A	1	MET	5.3
1	B	482	GLU	5.1
1	A	296	LYS	5.0
1	B	328	LYS	4.9
1	B	479	LEU	4.9
1	A	441	LYS	4.8
1	B	243	GLY	4.7
1	A	295	ARG	4.6
1	B	245	THR	4.4
1	B	326	GLY	4.2
1	B	239	ILE	4.1
1	B	465	ASP	4.0
1	A	243	GLY	3.9
1	A	242	ASN	3.9
1	B	299	ARG	3.9
1	A	328	LYS	3.8
1	A	445	LYS	3.7
1	B	289	ASN	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	514	PRO	3.6
1	B	516	ARG	3.5
1	A	244	LYS	3.5
1	B	463	ARG	3.4
1	B	448	GLU	3.4
1	A	294	GLN	3.3
1	B	453	TYR	3.3
1	B	439	MET	3.2
1	B	329	LYS	3.2
1	B	295	ARG	3.1
1	A	480	GLY	3.1
1	B	480	GLY	3.1
1	B	294	GLN	3.0
1	A	99	GLU	3.0
1	A	463	ARG	2.9
1	A	166	ARG	2.9
1	A	363	ILE	2.9
1	B	32	ASP	2.8
1	B	412	SER	2.8
1	A	179	LYS	2.8
1	A	370	ARG	2.8
1	B	395	ASP	2.7
1	A	293	LEU	2.7
1	A	559	GLU	2.7
1	B	342	VAL	2.7
1	B	166	ARG	2.6
1	A	299	ARG	2.6
1	A	513	LEU	2.5
1	B	558	LYS	2.5
1	A	300	ILE	2.5
1	B	179	LYS	2.5
1	A	336	LYS	2.4
1	A	465	ASP	2.4
1	A	95	ARG	2.4
1	B	458	LEU	2.4
1	A	77	GLY	2.3
1	A	483	GLY	2.3
1	B	363	ILE	2.3
1	A	516	ARG	2.3
1	A	252	HIS	2.3
1	A	344	LYS	2.3
1	B	325	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	263	GLU	2.2
1	A	482	GLU	2.1
1	B	514	PRO	2.1
1	B	472	PHE	2.1
1	B	376	VAL	2.1
1	B	413	ALA	2.1
1	B	285	LYS	2.1
1	B	421	GLU	2.1
1	B	417	GLU	2.1
1	A	329	LYS	2.0
1	A	326	GLY	2.0
1	B	99	GLU	2.0
1	A	412	SER	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	CD	A	601	1/1	0.99	0.02	19,19,19,19	0
2	CD	B	602	1/1	1.00	0.02	25,25,25,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.