



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:09 PM UTC

PDB ID : 1Q7Z / pdb_00001q7z
Title : Cobalamin-dependent methionine synthase (1-566) from *Thermotoga maritima* (Cd²⁺ 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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

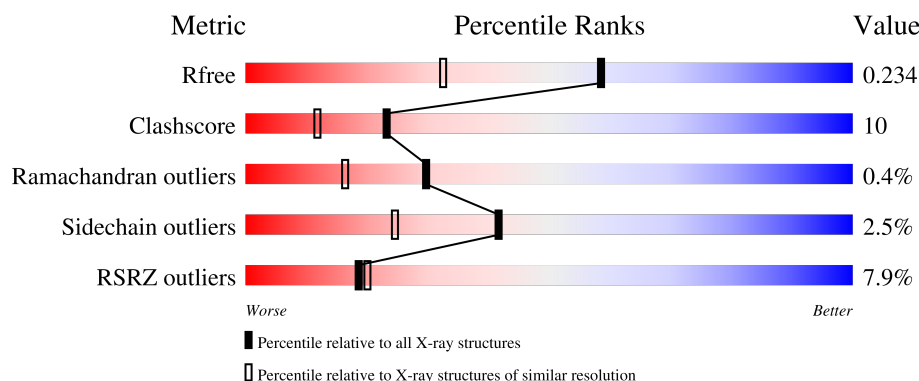
1 Overall quality at a glance

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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 ≥ 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	6% 76% 21% ..
1	B	566	10% 71% 22% ..

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
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 CADMIUM ION (CCD ID: CD) (formula: Cd).

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

- Molecule 3 is water.

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

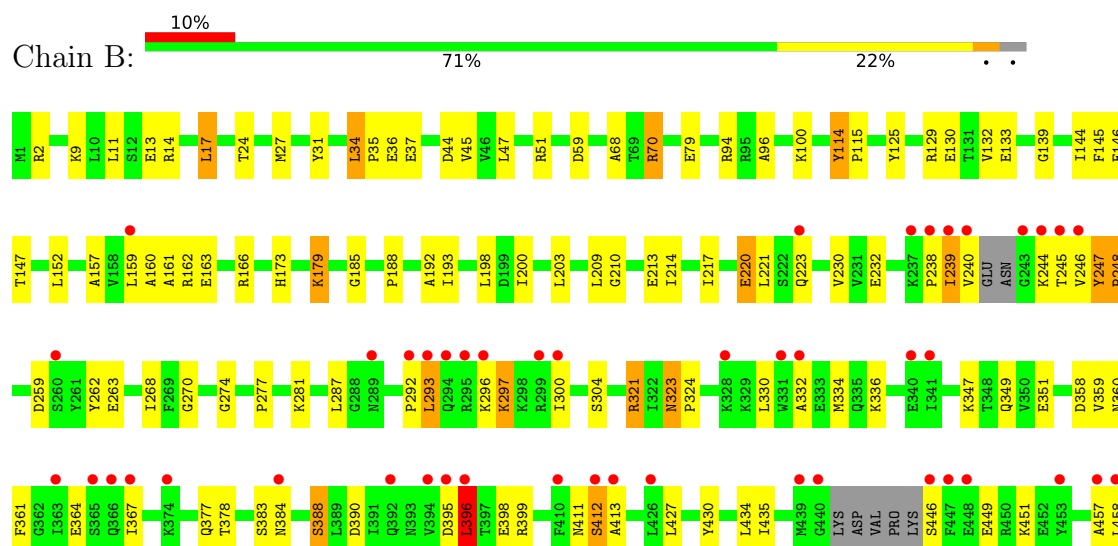
3 Residue-property plots

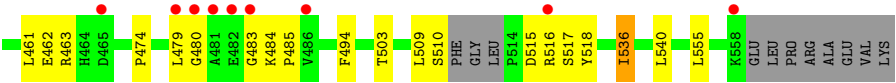
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



- 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, α , β , γ	59.54Å 85.13Å 125.61Å 90.00° 100.86° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 20.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.70) 96.2 (20.00-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 1.65Å)	Xtriage
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 ²)	22.0	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9111	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 ⓘ

5.1 Standard geometry ⓘ

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	0.36	0/4505	0.93	21/6083 (0.3%)
1	B	0.33	0/4411	0.91	19/5951 (0.3%)
All	All	0.35	0/8916	0.92	40/12034 (0.3%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	247	TYR	CA-C-N	9.70	129.95	119.87
1	B	247	TYR	C-N-CA	9.70	129.95	119.87
1	A	413	ALA	N-CA-C	-9.14	93.31	108.76
1	A	321	ARG	N-CA-C	8.85	122.04	111.33
1	B	321	ARG	N-CA-C	8.71	122.90	111.75
1	A	247	TYR	CA-C-N	7.74	129.04	120.45
1	A	247	TYR	C-N-CA	7.74	129.04	120.45
1	A	248	PRO	N-CA-C	7.36	123.55	114.35
1	B	378	THR	N-CA-C	7.25	118.97	111.14
1	A	378	THR	N-CA-C	6.92	118.61	111.14
1	A	412	SER	N-CA-C	6.53	124.71	110.80
1	A	536	ILE	N-CA-C	-6.37	97.80	107.73
1	B	248	PRO	N-CA-C	6.31	121.80	114.03
1	B	536	ILE	N-CA-C	-6.26	99.28	108.54
1	B	68	ALA	N-CA-C	6.20	118.92	109.62
1	A	411	ASN	N-CA-C	6.16	118.02	109.15
1	A	41	LYS	N-CA-C	6.13	118.05	111.36
1	A	68	ALA	N-CA-C	6.06	118.71	109.62
1	A	185	GLY	N-CA-C	5.97	123.69	115.27
1	A	505	GLY	N-CA-C	-5.88	99.23	113.18
1	A	114	TYR	N-CA-C	-5.80	102.28	109.64
1	B	114	TYR	N-CA-C	-5.65	102.46	109.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	323	ASN	CA-C-N	5.64	125.48	119.28
1	B	323	ASN	C-N-CA	5.64	125.48	119.28
1	A	304	SER	N-CA-C	5.56	117.24	108.96
1	B	304	SER	N-CA-C	5.54	117.22	108.96
1	B	34	LEU	N-CA-C	-5.47	101.61	109.48
1	B	185	GLY	N-CA-C	5.38	122.86	115.27
1	A	110	GLY	N-CA-C	-5.33	107.96	115.32
1	A	506	LEU	N-CA-C	5.30	117.47	111.11
1	A	119	THR	N-CA-C	5.24	118.15	109.46
1	B	146	GLU	N-CA-C	5.19	118.67	109.96
1	A	34	LEU	N-CA-C	-5.17	102.36	109.71
1	B	139	GLY	N-CA-C	5.17	123.56	115.08
1	A	116	LEU	N-CA-C	-5.11	105.79	111.36
1	A	104	GLY	N-CA-C	-5.10	104.61	111.54
1	B	388	SER	N-CA-C	-5.08	99.00	107.99
1	B	396	LEU	N-CA-C	-5.03	105.90	112.23
1	B	210	GLY	CA-C-N	5.00	125.03	119.32
1	B	210	GLY	C-N-CA	5.00	125.03	119.32

There are no chirality outliers.

There are no planarity outliers.

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	4423	0	4510	93	0
1	B	4334	0	4421	91	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
All	All	9111	0	8931	182	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 (182) 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:1:MET:HE3	1:A:139:GLY:HA3	1.78	0.65
1:A:412:SER:HA	1:A:435:ILE:O	1.95	0.65
1:B:24:THR:HA	1:B:27:MET:HE3	1.78	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:B:413:ALA:HB2	1:B:434:LEU:HD11	1.85	0.59
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1:MET:HE3	1:A:139:GLY:CA	2.36	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:509:LEU:C	1:A:509:LEU:HD13	2.37	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:446:SER:HG	1:B:449:GLU:HG3	1.77	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:HD13	1:A:509:LEU:O	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:A:321:ARG:HB2	1:A:349:GLN:CD	2.41	0.45
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
1:B:246:VAL:O	1:B:248:PRO:HD3	2.17	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:321:ARG:HB2	1:B:349:GLN:CD	2.44	0.43
1:B:364:GLU:HB3	1:B:396:LEU:HD12	2.00	0.43
1:A:512:GLY:C	1:A:513:LEU:HD23	2.44	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: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:223:GLN:HB3	1:A:298:LYS:NZ	2.35	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
1:B:232:GLU:HA	1:B:270:GLY:O	2.20	0.41
1:B:395:ASP:OD1	1:B:395:ASP:C	2.62	0.41

Continued on next page...

Continued from previous page...

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

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%)	535 (96%)	21 (4%)	1 (0%)	43	28
1	B	540/566 (95%)	518 (96%)	19 (4%)	3 (1%)	21	9
All	All	1097/1132 (97%)	1053 (96%)	40 (4%)	4 (0%)	30	16

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 ⓘ

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%)	51	36
1	B	478/494 (97%)	463 (97%)	15 (3%)	35	18
All	All	966/988 (98%)	942 (98%)	24 (2%)	42	24

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	ARG
1	A	18	LEU
1	A	147	THR
1	A	248	PRO
1	A	366	GLN
1	A	463	ARG
1	A	513	LEU
1	A	558	LYS
1	B	17	LEU
1	B	70	ARG
1	B	94	ARG
1	B	147	THR
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	335	GLN
1	A	425	ASN
1	B	257	HIS
1	B	294	GLN
1	B	335	GLN
1	B	349	GLN
1	B	366	GLN

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 oligosaccharides 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

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, 95th 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 ²)	Q<0.9
1	A	559/566 (98%)	0.38	32 (5%)	29 32	13, 24, 44, 54	0
1	B	548/566 (96%)	0.63	55 (10%)	12 13	16, 29, 47, 58	0
All	All	1107/1132 (97%)	0.50	87 (7%)	18 20	13, 26, 46, 58	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	511	PHE	7.9
1	A	483	GLY	5.0
1	A	512	GLY	5.0
1	A	513	LEU	4.9
1	A	1	MET	4.5
1	B	412	SER	4.4
1	A	442	ASP	4.3
1	B	395	ASP	4.2
1	A	296	LYS	4.2
1	A	293	LEU	4.1
1	B	243	GLY	4.1
1	B	479	LEU	4.1
1	B	440	GLY	4.0
1	B	239	ILE	3.9
1	A	328	LYS	3.4
1	B	413	ALA	3.3
1	A	463	ARG	3.3
1	A	421	GLU	3.3
1	A	300	ILE	3.2
1	B	295	ARG	3.2
1	A	412	SER	3.2
1	A	240	VAL	3.1
1	B	293	LEU	3.1
1	B	244	LYS	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	369	VAL	3.0
1	A	443	VAL	3.0
1	A	441	LYS	2.9
1	B	240	VAL	2.9
1	B	367	ILE	2.9
1	B	516	ARG	2.8
1	A	445	LYS	2.8
1	B	482	GLU	2.8
1	B	296	LYS	2.8
1	B	448	GLU	2.7
1	A	514	PRO	2.7
1	B	237	LYS	2.7
1	A	480	GLY	2.7
1	B	365	SER	2.7
1	B	289	ASN	2.7
1	B	384	ASN	2.7
1	B	439	MET	2.7
1	A	559	GLU	2.7
1	B	363	ILE	2.7
1	B	453	TYR	2.6
1	B	458	LEU	2.6
1	A	295	ARG	2.6
1	B	245	THR	2.6
1	B	480	GLY	2.6
1	B	447	PHE	2.6
1	A	363	ILE	2.6
1	B	446	SER	2.5
1	A	14	ARG	2.5
1	B	457	ALA	2.5
1	B	328	LYS	2.5
1	B	396	LEU	2.5
1	B	341	ILE	2.5
1	B	558	LYS	2.5
1	B	486	VAL	2.4
1	A	336	LYS	2.4
1	B	331	TRP	2.4
1	A	243	GLY	2.4
1	B	260	SER	2.3
1	B	374	LYS	2.3
1	B	300	ILE	2.3
1	B	246	VAL	2.3
1	A	365	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	410	PHE	2.3
1	B	426	LEU	2.3
1	A	244	LYS	2.3
1	A	77	GLY	2.3
1	B	159	LEU	2.2
1	B	340	GLU	2.2
1	A	516	ARG	2.2
1	B	332	ALA	2.2
1	B	481	ALA	2.2
1	B	465	ASP	2.1
1	A	289	ASN	2.1
1	B	392	GLN	2.1
1	B	483	GLY	2.1
1	B	223	GLN	2.1
1	B	366	GLN	2.1
1	B	238	PRO	2.1
1	B	394	VAL	2.1
1	B	299	ARG	2.1
1	B	292	PRO	2.1
1	B	294	GLN	2.0
1	A	246	VAL	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 oligosaccharides 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, 95th 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($\text{\AA}^2$)	Q<0.9
2	CD	A	601	1/1	0.99	0.03	19,19,19,19	0
2	CD	B	602	1/1	0.99	0.02	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.