



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:17 AM UTC

PDB ID : 2E0K / pdb_00002e0k
Title : Crystal structure of CbiL, a methyltransferase involved in anaerobic vitamin B12 biosynthesis
Authors : Wada, K.; Fukuyama, K.
Deposited on : 2006-10-10
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

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

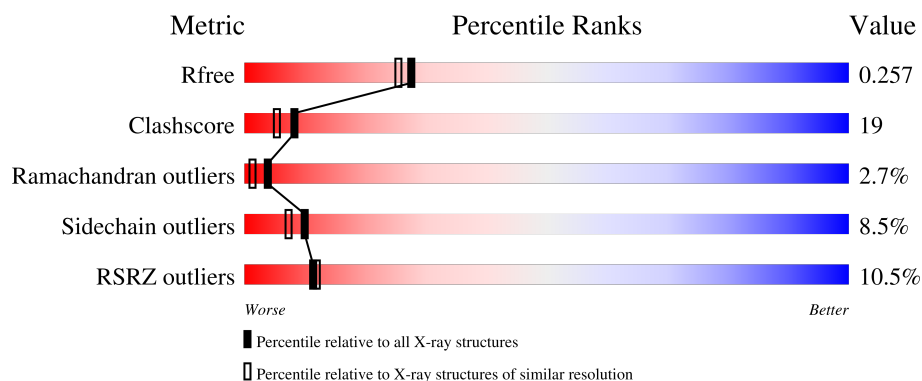
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 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	259	12% 63% 26% 7%
1	B	259	7% 62% 26% 5% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3754 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 Precorrin-2 C20-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1794	1132	305	345	12			
1	B	244	Total	C	N	O	S	0	0	0
			1809	1140	308	350	11			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	247	LYS	-	cloning artifact	UNP Q8KFD9
A	248	LEU	-	cloning artifact	UNP Q8KFD9
A	249	ALA	-	cloning artifact	UNP Q8KFD9
A	250	ALA	-	cloning artifact	UNP Q8KFD9
A	251	ALA	-	cloning artifact	UNP Q8KFD9
A	252	LEU	-	cloning artifact	UNP Q8KFD9
A	253	GLU	-	cloning artifact	UNP Q8KFD9
A	254	HIS	-	expression tag	UNP Q8KFD9
A	255	HIS	-	expression tag	UNP Q8KFD9
A	256	HIS	-	expression tag	UNP Q8KFD9
A	257	HIS	-	expression tag	UNP Q8KFD9
A	258	HIS	-	expression tag	UNP Q8KFD9
A	259	HIS	-	expression tag	UNP Q8KFD9
B	247	LYS	-	cloning artifact	UNP Q8KFD9
B	248	LEU	-	cloning artifact	UNP Q8KFD9
B	249	ALA	-	cloning artifact	UNP Q8KFD9
B	250	ALA	-	cloning artifact	UNP Q8KFD9
B	251	ALA	-	cloning artifact	UNP Q8KFD9
B	252	LEU	-	cloning artifact	UNP Q8KFD9
B	253	GLU	-	cloning artifact	UNP Q8KFD9
B	254	HIS	-	expression tag	UNP Q8KFD9
B	255	HIS	-	expression tag	UNP Q8KFD9
B	256	HIS	-	expression tag	UNP Q8KFD9
B	257	HIS	-	expression tag	UNP Q8KFD9
B	258	HIS	-	expression tag	UNP Q8KFD9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	259	HIS	-	expression tag	UNP Q8KFD9

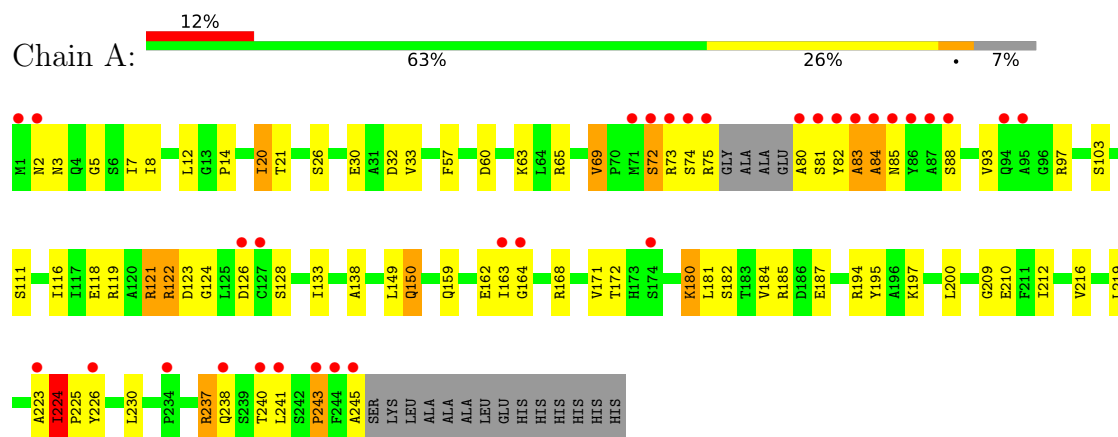
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	74	Total O 74 74	0	0
2	B	77	Total O 77 77	0	0

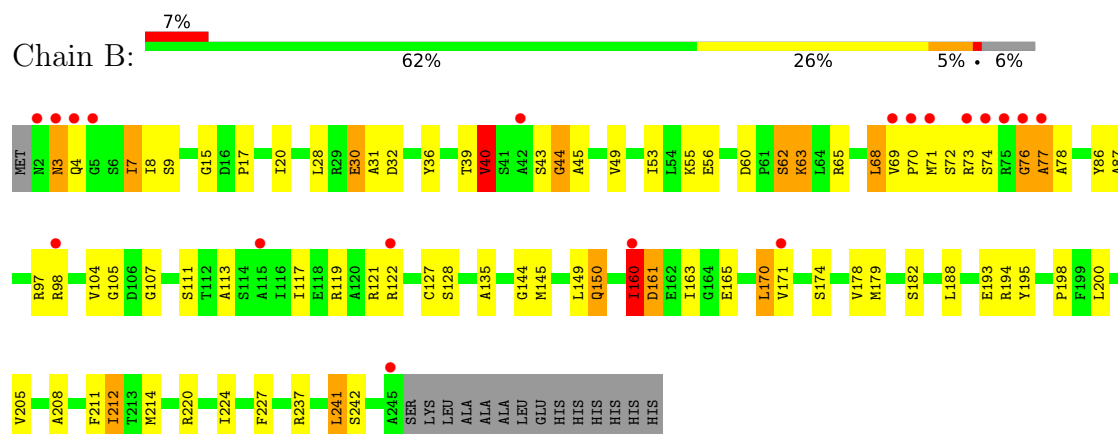
3 Residue-property plots

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: Precorrin-2 C20-methyltransferase



• Molecule 1: Precorrin-2 C20-methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	88.21Å 88.21Å 123.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 50.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.10) 99.8 (50.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.28 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.218 , 0.273 0.212 , 0.257	Depositor DCC
R_{free} test set	1478 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3754	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 4.29% 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 ⓘ

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	1.27	7/1822 (0.4%)	1.24	7/2469 (0.3%)
1	B	1.35	8/1838 (0.4%)	1.23	9/2493 (0.4%)
All	All	1.31	15/3660 (0.4%)	1.24	16/4962 (0.3%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	ARG	CZ-NH2	12.41	1.49	1.33
1	A	72	SER	C-N	9.95	1.46	1.33
1	B	20	ILE	CA-CB	7.11	1.62	1.54
1	A	73	ARG	NE-CZ	7.04	1.40	1.33
1	B	97	ARG	CZ-NH1	6.79	1.42	1.32
1	A	116	ILE	CA-CB	6.38	1.62	1.54
1	B	208	ALA	CA-CB	5.82	1.62	1.53
1	B	135	ALA	CA-CB	5.38	1.61	1.53
1	A	33	VAL	CA-CB	5.38	1.62	1.54
1	B	214	MET	N-CA	-5.18	1.39	1.46
1	B	113	ALA	CA-CB	-5.12	1.45	1.53
1	A	111	SER	C-O	-5.09	1.17	1.23
1	A	103	SER	CA-C	-5.06	1.46	1.52
1	B	174	SER	CA-C	5.05	1.59	1.52
1	B	211	PHE	C-O	-5.03	1.18	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	ARG	NE-CZ-NH1	-9.20	112.30	121.50
1	A	73	ARG	NE-CZ-NH2	7.40	125.86	119.20
1	B	224	ILE	O-C-N	7.13	125.86	121.37
1	A	57	PHE	N-CA-C	6.99	121.90	112.88
1	B	188	LEU	N-CA-C	6.93	118.49	111.07
1	B	145	MET	CA-C-N	-6.57	113.17	120.14
1	B	145	MET	C-N-CA	-6.57	113.17	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	170	LEU	N-CA-C	6.54	118.96	111.11
1	B	171	VAL	N-CA-C	6.41	119.10	111.09
1	B	242	SER	N-CA-C	6.05	117.70	110.07
1	A	121	ARG	O-C-N	-5.88	115.45	122.15
1	B	105	GLY	N-CA-C	-5.67	104.54	111.35
1	A	121	ARG	CA-C-N	5.49	128.40	120.38
1	A	121	ARG	C-N-CA	5.49	128.40	120.38
1	A	224	ILE	CB-CA-C	5.37	117.17	110.95
1	B	40	VAL	CB-CA-C	-5.30	102.72	110.62

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	1794	0	1822	69	0
1	B	1809	0	1830	73	0
2	A	74	0	0	4	0
2	B	77	0	0	7	0
All	All	3754	0	3652	140	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 19.

All (140) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:LYS:CE	1:A:182:SER:HB2	1.82	1.10
1:A:180:LYS:NZ	1:A:182:SER:HB2	1.69	1.07
1:B:9:SER:HB2	1:B:117:ILE:HD11	1.37	1.06
1:A:180:LYS:O	1:A:180:LYS:HG3	1.57	1.03
1:B:3:ASN:HB2	1:B:98:ARG:HB3	1.40	1.03
1:A:224:ILE:HD13	1:A:224:ILE:H	1.27	0.98
1:A:163:ILE:HD13	1:A:184:VAL:HG11	1.45	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ARG:HG3	1:A:237:ARG:HH11	1.30	0.96
1:B:73:ARG:HH11	1:B:76:GLY:CA	1.82	0.92
1:A:168:ARG:O	1:A:171:VAL:HG22	1.70	0.89
1:B:160:ILE:HG12	1:B:178:VAL:CG1	2.02	0.88
1:A:180:LYS:NZ	1:A:182:SER:CB	2.40	0.85
1:A:75:ARG:HH21	1:A:80:ALA:HB1	1.43	0.82
1:B:73:ARG:HH11	1:B:76:GLY:HA2	1.45	0.82
1:B:160:ILE:HG12	1:B:178:VAL:HG11	1.62	0.82
1:A:171:VAL:HG23	1:A:172:THR:HG23	1.62	0.81
1:A:185:ARG:HB2	1:A:224:ILE:CG1	2.11	0.79
1:A:180:LYS:HE2	1:A:182:SER:HB2	1.62	0.77
1:B:73:ARG:NH1	1:B:76:GLY:HA2	2.00	0.77
1:B:200:LEU:HD11	1:B:212:ILE:HG23	1.67	0.76
1:B:194:ARG:HH21	1:B:194:ARG:HB2	1.50	0.75
1:B:9:SER:CB	1:B:117:ILE:HD11	2.15	0.74
1:B:160:ILE:CG1	1:B:178:VAL:CG1	2.65	0.73
1:A:224:ILE:H	1:A:224:ILE:CD1	2.02	0.72
1:B:60:ASP:H	1:B:63:LYS:NZ	1.88	0.71
1:A:5:GLY:O	1:A:93:VAL:HG13	1.92	0.69
1:A:163:ILE:HD13	1:A:184:VAL:CG1	2.22	0.69
1:A:184:VAL:HG12	1:A:184:VAL:O	1.93	0.69
1:B:60:ASP:OD1	1:B:62:SER:HB3	1.94	0.68
1:B:3:ASN:HA	1:B:30:GLU:O	1.94	0.68
1:A:8:ILE:HD13	2:A:311:HOH:O	1.92	0.67
1:B:194:ARG:HB2	1:B:194:ARG:NH2	2.09	0.67
1:B:49:VAL:HG23	1:B:104:VAL:HG21	1.78	0.66
1:A:119:ARG:HA	1:A:122:ARG:HD3	1.76	0.66
1:A:159:GLN:HG2	1:A:180:LYS:HG2	1.76	0.66
1:B:212:ILE:HG22	1:B:241:LEU:HD21	1.76	0.66
1:B:72:SER:C	2:B:296:HOH:O	2.39	0.65
1:B:73:ARG:NH1	1:B:76:GLY:CA	2.57	0.65
1:A:185:ARG:HB2	1:A:224:ILE:HG12	1.77	0.65
1:A:159:GLN:HA	1:A:180:LYS:HG2	1.79	0.64
1:B:198:PRO:HG3	1:B:237:ARG:NH1	2.13	0.64
1:B:36:TYR:HD1	2:B:321:HOH:O	1.80	0.63
1:B:76:GLY:O	1:B:78:ALA:N	2.31	0.63
1:A:8:ILE:CD1	2:A:311:HOH:O	2.45	0.63
1:A:200:LEU:HD11	1:A:212:ILE:CG2	2.27	0.63
1:A:75:ARG:NH2	1:A:80:ALA:HB1	2.14	0.63
1:B:8:ILE:HD12	1:B:98:ARG:CZ	2.29	0.63
1:B:119:ARG:HH22	1:B:122:ARG:HH11	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:LYS:HZ3	1:A:182:SER:CB	2.12	0.61
1:B:212:ILE:HG22	1:B:241:LEU:CD2	2.30	0.61
1:A:185:ARG:CB	1:A:224:ILE:HG12	2.31	0.61
1:A:32:ASP:HB3	1:A:97:ARG:HD2	1.83	0.61
1:B:73:ARG:HH11	1:B:76:GLY:HA3	1.63	0.61
1:B:200:LEU:HD11	1:B:212:ILE:CG2	2.30	0.60
1:A:180:LYS:HD2	1:A:226:TYR:CE1	2.36	0.60
1:A:163:ILE:CD1	1:A:184:VAL:HG11	2.27	0.59
1:B:205:VAL:HG22	1:B:212:ILE:HD11	1.84	0.59
1:B:49:VAL:HG21	1:B:227:PHE:CZ	2.36	0.59
1:A:180:LYS:HZ1	1:A:182:SER:HB2	1.66	0.59
1:B:76:GLY:C	1:B:78:ALA:H	2.11	0.59
1:A:180:LYS:HZ3	1:A:182:SER:HB2	1.63	0.59
1:B:193:GLU:OE2	1:B:220:ARG:NH1	2.21	0.58
1:A:180:LYS:HZ1	1:A:182:SER:CB	2.16	0.58
1:B:160:ILE:HD11	1:B:179:MET:O	2.02	0.58
1:A:162:GLU:HG2	1:A:164:GLY:H	1.67	0.58
1:A:121:ARG:O	1:A:123:ASP:O	2.22	0.58
1:A:200:LEU:HD11	1:A:212:ILE:HG23	1.85	0.58
1:B:76:GLY:C	1:B:78:ALA:N	2.58	0.57
1:B:60:ASP:O	1:B:63:LYS:HG2	2.04	0.57
1:B:241:LEU:HD12	1:B:241:LEU:N	2.20	0.57
1:A:224:ILE:HD13	1:A:224:ILE:N	2.10	0.57
1:A:185:ARG:CB	1:A:224:ILE:CG1	2.82	0.57
1:B:60:ASP:H	1:B:63:LYS:HZ2	1.53	0.56
1:A:26:SER:O	1:A:30:GLU:HG3	2.05	0.56
1:A:123:ASP:OD1	1:A:124:GLY:N	2.35	0.56
1:B:15:GLY:HA2	1:B:53:ILE:HD11	1.88	0.56
1:B:161:ASP:OD2	1:B:165:GLU:OE2	2.23	0.55
1:B:121:ARG:NH2	2:B:293:HOH:O	2.29	0.55
1:B:3:ASN:HB2	1:B:98:ARG:CB	2.26	0.55
1:A:83:ALA:HA	2:A:333:HOH:O	2.06	0.55
1:B:74:SER:N	2:B:296:HOH:O	2.32	0.54
1:A:181:LEU:HD11	1:A:230:LEU:HB2	1.89	0.54
1:B:73:ARG:N	2:B:296:HOH:O	2.40	0.54
1:A:237:ARG:HH11	1:A:237:ARG:CG	2.14	0.54
1:A:60:ASP:O	1:A:63:LYS:HB2	2.08	0.54
1:B:241:LEU:N	1:B:241:LEU:CD1	2.71	0.53
1:B:160:ILE:HG13	1:B:178:VAL:HG13	1.90	0.53
1:A:240:THR:HG23	1:B:121:ARG:HD3	1.92	0.52
1:A:182:SER:OG	1:A:226:TYR:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ALA:HA	2:B:279:HOH:O	2.11	0.51
1:B:7:ILE:O	1:B:127:CYS:HA	2.11	0.51
1:A:238:GLN:HG3	2:A:294:HOH:O	2.10	0.51
1:B:49:VAL:O	1:B:53:ILE:HG12	2.12	0.50
1:A:209:GLY:O	1:A:210:GLU:C	2.54	0.49
1:B:40:VAL:HG22	1:B:68:LEU:HG	1.94	0.49
1:A:69:VAL:HG13	1:A:80:ALA:HA	1.95	0.48
1:B:194:ARG:NH2	1:B:194:ARG:CB	2.77	0.47
1:B:39:THR:HA	1:B:69:VAL:O	2.14	0.47
1:A:14:PRO:HG3	1:A:138:ALA:HB2	1.97	0.47
1:B:17:PRO:HG3	1:B:56:GLU:HG3	1.97	0.47
1:B:60:ASP:H	1:B:63:LYS:HZ3	1.60	0.47
1:A:74:SER:HA	1:A:80:ALA:HB3	1.97	0.47
1:B:119:ARG:HH22	1:B:122:ARG:NH1	2.13	0.47
1:A:184:VAL:CG1	1:A:184:VAL:O	2.63	0.46
1:B:60:ASP:HB3	1:B:63:LYS:HD3	1.97	0.46
1:B:32:ASP:OD1	1:B:98:ARG:N	2.38	0.46
1:A:75:ARG:HB3	1:A:81:SER:HA	1.97	0.46
1:B:73:ARG:NE	1:B:73:ARG:HA	2.29	0.46
1:A:226:TYR:C	1:A:226:TYR:CD2	2.93	0.46
1:A:243:PRO:C	1:A:245:ALA:H	2.22	0.46
1:B:198:PRO:HG3	1:B:237:ARG:CZ	2.46	0.46
1:B:170:LEU:HD13	1:B:195:TYR:CE2	2.50	0.45
1:A:20:ILE:HD12	1:A:21:THR:H	1.81	0.45
1:B:49:VAL:CG2	1:B:227:PHE:CZ	2.99	0.45
1:B:160:ILE:CG1	1:B:178:VAL:HG13	2.41	0.45
1:B:49:VAL:CG2	1:B:104:VAL:HG21	2.44	0.45
1:A:224:ILE:CD1	1:A:224:ILE:N	2.76	0.44
1:B:212:ILE:CG2	1:B:241:LEU:HD21	2.46	0.44
1:B:149:LEU:O	1:B:150:GLN:C	2.59	0.44
1:B:160:ILE:HG13	1:B:178:VAL:CG1	2.45	0.44
1:B:160:ILE:HD12	1:B:160:ILE:N	2.32	0.44
1:B:4:GLN:HB3	1:B:30:GLU:CD	2.43	0.44
1:A:14:PRO:HD3	1:A:133:ILE:HB	2.00	0.44
1:B:43:SER:O	1:B:44:GLY:O	2.36	0.44
1:A:185:ARG:HB2	1:A:224:ILE:HG13	1.97	0.44
1:A:7:ILE:O	1:A:8:ILE:HD13	2.17	0.44
1:A:12:LEU:C	1:A:20:ILE:HD13	2.43	0.43
1:A:195:TYR:CE1	1:A:197:LYS:HD2	2.54	0.43
1:A:8:ILE:HD12	1:A:128:SER:OG	2.19	0.42
1:A:82:TYR:C	1:A:84:ALA:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ASN:O	1:A:88:SER:HB3	2.20	0.42
1:B:107:GLY:O	1:B:111:SER:HB3	2.18	0.42
1:A:223:ALA:O	1:A:225:PRO:HD3	2.19	0.42
1:A:121:ARG:NH1	1:B:144:GLY:O	2.52	0.41
1:B:73:ARG:CA	2:B:296:HOH:O	2.69	0.41
1:A:185:ARG:HB2	1:A:224:ILE:CD1	2.51	0.41
1:B:31:ALA:HA	1:B:98:ARG:HG3	2.03	0.41
1:A:163:ILE:HD12	1:A:163:ILE:HA	1.98	0.40
1:B:86:TYR:O	1:B:87:ALA:C	2.65	0.40
1:A:149:LEU:O	1:A:150:GLN:C	2.64	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	237/259 (92%)	216 (91%)	15 (6%)	6 (2%)	4	1
1	B	242/259 (93%)	225 (93%)	10 (4%)	7 (3%)	3	1
All	All	479/518 (92%)	441 (92%)	25 (5%)	13 (3%)	4	1

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	ALA
1	A	150	GLN
1	B	77	ALA
1	B	44	GLY
1	B	76	GLY
1	B	160	ILE
1	A	3	ASN
1	A	83	ALA

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Mol	Chain	Res	Type
1	B	150	GLN
1	A	72	SER
1	B	45	ALA
1	B	70	PRO
1	A	243	PRO

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	194/206 (94%)	179 (92%)	15 (8%)	12	9
1	B	194/206 (94%)	176 (91%)	18 (9%)	8	6
All	All	388/412 (94%)	355 (92%)	33 (8%)	10	7

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	20	ILE
1	A	65	ARG
1	A	69	VAL
1	A	118	GLU
1	A	122	ARG
1	A	126	ASP
1	A	180	LYS
1	A	187	GLU
1	A	194	ARG
1	A	216	VAL
1	A	219	LEU
1	A	224	ILE
1	A	237	ARG
1	A	241	LEU
1	B	3	ASN
1	B	7	ILE
1	B	28	LEU

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Mol	Chain	Res	Type
1	B	30	GLU
1	B	40	VAL
1	B	55	LYS
1	B	62	SER
1	B	63	LYS
1	B	65	ARG
1	B	68	LEU
1	B	71	MET
1	B	128	SER
1	B	160	ILE
1	B	161	ASP
1	B	163	ILE
1	B	182	SER
1	B	212	ILE
1	B	241	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	85	ASN
1	A	150	GLN
1	A	159	GLN
1	A	238	GLN
1	B	3	ASN
1	B	94	GLN
1	B	173	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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, 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	241/259 (93%)	0.77	32 (13%) 7 7	5, 29, 53, 70	0
1	B	244/259 (94%)	0.49	19 (7%) 19 20	4, 23, 48, 66	0
All	All	485/518 (93%)	0.63	51 (10%) 11 12	4, 26, 53, 70	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	80	ALA	6.1
1	A	86	TYR	5.7
1	B	5	GLY	5.3
1	A	87	ALA	5.0
1	B	98	ARG	4.7
1	A	82	TYR	4.6
1	A	72	SER	4.5
1	B	76	GLY	4.5
1	A	83	ALA	4.3
1	A	244	PHE	4.2
1	B	4	GLN	4.2
1	A	85	ASN	4.1
1	A	245	ALA	4.0
1	A	74	SER	3.8
1	A	84	ALA	3.8
1	A	73	ARG	3.7
1	A	81	SER	3.5
1	A	126	ASP	3.4
1	B	3	ASN	3.3
1	A	1	MET	3.3
1	A	241	LEU	3.3
1	B	160	ILE	3.1
1	B	245	ALA	3.1
1	B	77	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	75	ARG	2.9
1	A	75	ARG	2.9
1	A	2	ASN	2.9
1	A	238	GLN	2.8
1	B	73	ARG	2.8
1	B	70	PRO	2.7
1	A	223	ALA	2.7
1	A	163	ILE	2.6
1	B	122	ARG	2.6
1	B	69	VAL	2.5
1	A	240	THR	2.5
1	A	234	PRO	2.5
1	B	74	SER	2.5
1	B	42	ALA	2.5
1	B	2	ASN	2.5
1	B	115	ALA	2.4
1	B	71	MET	2.4
1	A	164	GLY	2.4
1	A	174	SER	2.3
1	A	243	PRO	2.3
1	A	71	MET	2.3
1	A	95	ALA	2.2
1	A	226	TYR	2.2
1	A	94	GLN	2.1
1	B	171	VAL	2.1
1	A	127	CYS	2.0
1	A	88	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 oligosaccharides 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.