



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:45 PM UTC

PDB ID : 3B3D / pdb_00003b3d
Title : B.subtilis YtbE
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Deposited on : 2007-10-20
Resolution : 2.30 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

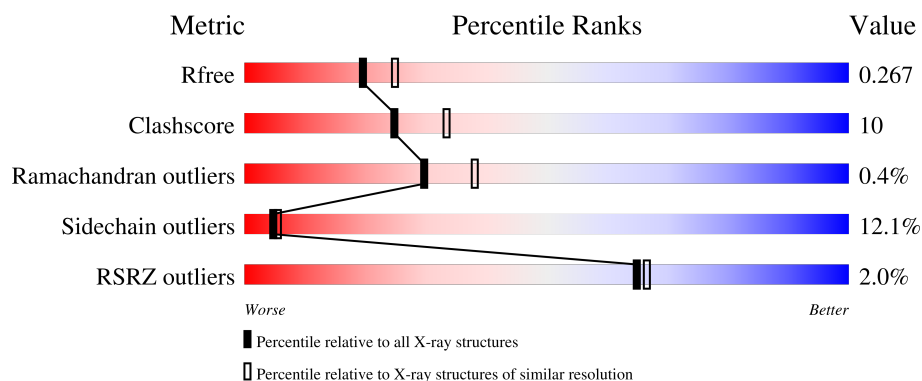
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	314	3% 64% 17% 6% • 11%
1	B	314	2% 69% 15% • 12%
1	C	314	% 68% 17% • • 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7067 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 Putative morphine dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	2	0
			2253	1432	382	431	8			
1	B	277	Total	C	N	O	S	0	6	0
			2271	1447	386	430	8			
1	C	280	Total	C	N	O	S	0	5	0
			2283	1454	387	433	9			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	expression tag	UNP O34678
A	-32	GLY	-	expression tag	UNP O34678
A	-31	SER	-	expression tag	UNP O34678
A	-30	SER	-	expression tag	UNP O34678
A	-29	HIS	-	expression tag	UNP O34678
A	-28	HIS	-	expression tag	UNP O34678
A	-27	HIS	-	expression tag	UNP O34678
A	-26	HIS	-	expression tag	UNP O34678
A	-25	HIS	-	expression tag	UNP O34678
A	-24	HIS	-	expression tag	UNP O34678
A	-23	SER	-	expression tag	UNP O34678
A	-22	SER	-	expression tag	UNP O34678
A	-21	GLY	-	expression tag	UNP O34678
A	-20	LEU	-	expression tag	UNP O34678
A	-19	VAL	-	expression tag	UNP O34678
A	-18	PRO	-	expression tag	UNP O34678
A	-17	ARG	-	expression tag	UNP O34678
A	-16	GLY	-	expression tag	UNP O34678
A	-15	SER	-	expression tag	UNP O34678
A	-14	HIS	-	expression tag	UNP O34678
A	-13	MET	-	expression tag	UNP O34678
A	-12	ALA	-	expression tag	UNP O34678
A	-11	SER	-	expression tag	UNP O34678

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP O34678
A	-9	THR	-	expression tag	UNP O34678
A	-8	GLY	-	expression tag	UNP O34678
A	-7	GLY	-	expression tag	UNP O34678
A	-6	GLN	-	expression tag	UNP O34678
A	-5	GLN	-	expression tag	UNP O34678
A	-4	MET	-	expression tag	UNP O34678
A	-3	GLY	-	expression tag	UNP O34678
A	-2	ARG	-	expression tag	UNP O34678
A	-1	GLY	-	expression tag	UNP O34678
A	0	SER	-	expression tag	UNP O34678
B	-33	MET	-	expression tag	UNP O34678
B	-32	GLY	-	expression tag	UNP O34678
B	-31	SER	-	expression tag	UNP O34678
B	-30	SER	-	expression tag	UNP O34678
B	-29	HIS	-	expression tag	UNP O34678
B	-28	HIS	-	expression tag	UNP O34678
B	-27	HIS	-	expression tag	UNP O34678
B	-26	HIS	-	expression tag	UNP O34678
B	-25	HIS	-	expression tag	UNP O34678
B	-24	HIS	-	expression tag	UNP O34678
B	-23	SER	-	expression tag	UNP O34678
B	-22	SER	-	expression tag	UNP O34678
B	-21	GLY	-	expression tag	UNP O34678
B	-20	LEU	-	expression tag	UNP O34678
B	-19	VAL	-	expression tag	UNP O34678
B	-18	PRO	-	expression tag	UNP O34678
B	-17	ARG	-	expression tag	UNP O34678
B	-16	GLY	-	expression tag	UNP O34678
B	-15	SER	-	expression tag	UNP O34678
B	-14	HIS	-	expression tag	UNP O34678
B	-13	MET	-	expression tag	UNP O34678
B	-12	ALA	-	expression tag	UNP O34678
B	-11	SER	-	expression tag	UNP O34678
B	-10	MET	-	expression tag	UNP O34678
B	-9	THR	-	expression tag	UNP O34678
B	-8	GLY	-	expression tag	UNP O34678
B	-7	GLY	-	expression tag	UNP O34678
B	-6	GLN	-	expression tag	UNP O34678
B	-5	GLN	-	expression tag	UNP O34678
B	-4	MET	-	expression tag	UNP O34678
B	-3	GLY	-	expression tag	UNP O34678

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	ARG	-	expression tag	UNP O34678
B	-1	GLY	-	expression tag	UNP O34678
B	0	SER	-	expression tag	UNP O34678
C	-33	MET	-	expression tag	UNP O34678
C	-32	GLY	-	expression tag	UNP O34678
C	-31	SER	-	expression tag	UNP O34678
C	-30	SER	-	expression tag	UNP O34678
C	-29	HIS	-	expression tag	UNP O34678
C	-28	HIS	-	expression tag	UNP O34678
C	-27	HIS	-	expression tag	UNP O34678
C	-26	HIS	-	expression tag	UNP O34678
C	-25	HIS	-	expression tag	UNP O34678
C	-24	HIS	-	expression tag	UNP O34678
C	-23	SER	-	expression tag	UNP O34678
C	-22	SER	-	expression tag	UNP O34678
C	-21	GLY	-	expression tag	UNP O34678
C	-20	LEU	-	expression tag	UNP O34678
C	-19	VAL	-	expression tag	UNP O34678
C	-18	PRO	-	expression tag	UNP O34678
C	-17	ARG	-	expression tag	UNP O34678
C	-16	GLY	-	expression tag	UNP O34678
C	-15	SER	-	expression tag	UNP O34678
C	-14	HIS	-	expression tag	UNP O34678
C	-13	MET	-	expression tag	UNP O34678
C	-12	ALA	-	expression tag	UNP O34678
C	-11	SER	-	expression tag	UNP O34678
C	-10	MET	-	expression tag	UNP O34678
C	-9	THR	-	expression tag	UNP O34678
C	-8	GLY	-	expression tag	UNP O34678
C	-7	GLY	-	expression tag	UNP O34678
C	-6	GLN	-	expression tag	UNP O34678
C	-5	GLN	-	expression tag	UNP O34678
C	-4	MET	-	expression tag	UNP O34678
C	-3	GLY	-	expression tag	UNP O34678
C	-2	ARG	-	expression tag	UNP O34678
C	-1	GLY	-	expression tag	UNP O34678
C	0	SER	-	expression tag	UNP O34678

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

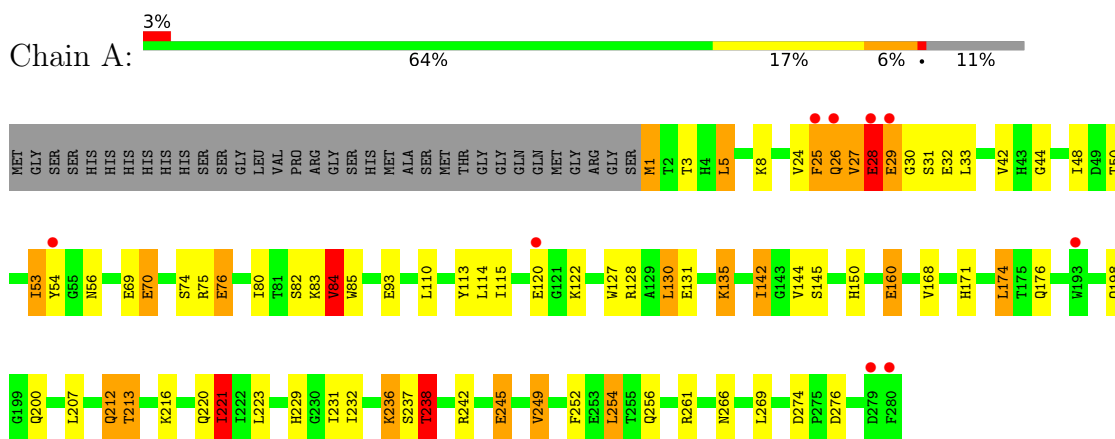
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	92	Total O 92 92	0	0
3	B	81	Total O 81 81	0	0
3	C	83	Total O 83 83	0	0

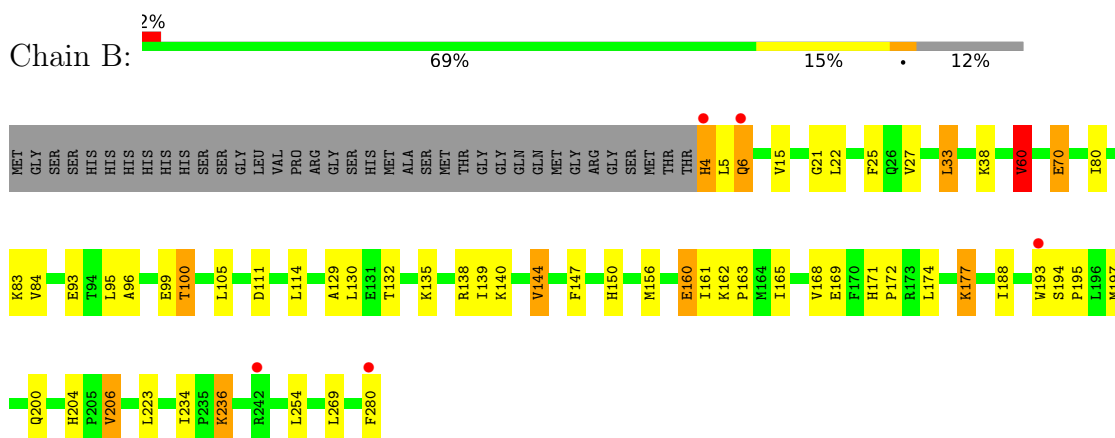
3 Residue-property plots [i](#)

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.

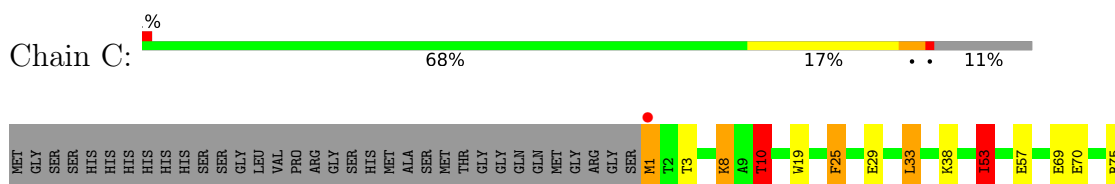
- Molecule 1: Putative morphine dehydrogenase

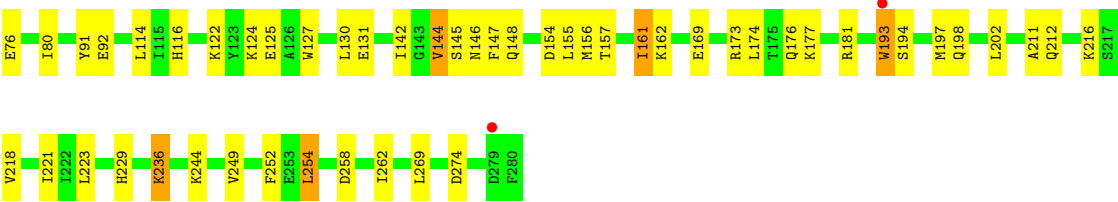


- Molecule 1: Putative morphine dehydrogenase



- Molecule 1: Putative morphine dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.11Å 89.17Å 115.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.2 (20.00-2.30) 97.0 (20.00-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.192 , 0.260 0.199 , 0.267	Depositor DCC
R_{free} test set	1898 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7067	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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: CA

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	1.04	3/2302 (0.1%)	1.17	9/3119 (0.3%)
1	B	1.04	7/2322 (0.3%)	1.09	1/3144 (0.0%)
1	C	0.97	3/2334 (0.1%)	1.09	5/3162 (0.2%)
All	All	1.02	13/6958 (0.2%)	1.12	15/9425 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	3	1
1	B	1	0
1	C	1	0
All	All	5	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	280	PHE	C-OXT	-9.86	1.03	1.23
1	A	232	ILE	CA-CB	6.32	1.61	1.54
1	C	221	ILE	CA-CB	6.30	1.61	1.54
1	B	60	VAL	CA-CB	6.01	1.62	1.54
1	A	80	ILE	CA-CB	5.97	1.61	1.54
1	B	80	ILE	CA-CB	5.93	1.61	1.54
1	B	165	ILE	CA-CB	5.55	1.62	1.54
1	B	15	VAL	CA-CB	5.52	1.61	1.54
1	C	10	THR	CA-CB	5.38	1.61	1.53
1	A	221	ILE	CA-CB	5.30	1.61	1.54
1	B	21	GLY	N-CA	5.29	1.50	1.45
1	C	80	ILE	CA-CB	5.14	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	168	VAL	CA-CB	5.13	1.62	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	84	VAL	CB-CA-C	-9.02	99.43	111.15
1	C	53	ILE	CB-CA-C	-8.13	96.26	111.79
1	A	238	THR	N-CA-C	-7.72	105.02	114.75
1	A	84	VAL	CB-CA-C	-7.71	101.13	111.15
1	C	10	THR	CB-CA-C	6.03	120.15	109.72
1	A	25	PHE	N-CA-C	-5.89	100.18	108.96
1	A	245	GLU	N-CA-C	5.68	117.47	111.28
1	A	274	ASP	CA-C-N	5.54	125.20	119.56
1	A	274	ASP	C-N-CA	5.54	125.20	119.56
1	A	84	VAL	N-CA-CB	5.32	116.33	110.53
1	A	249	VAL	CB-CA-C	5.27	119.93	111.29
1	C	274	ASP	CA-C-N	5.16	125.46	119.47
1	C	274	ASP	C-N-CA	5.16	125.46	119.47
1	C	244	LYS	N-CA-C	5.14	116.69	111.14
1	A	266	ASN	N-CA-C	5.08	117.84	110.42

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	26	GLN	CA
1	A	28	GLU	CA
1	A	142	ILE	CB
1	B	140[B]	LYS	CA
1	C	1	MET	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	27	VAL	Peptide

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	2253	0	2203	48	1
1	B	2271	0	2218	47	0
1	C	2283	0	2228	37	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	92	0	0	4	0
3	B	81	0	0	3	1
3	C	83	0	0	9	0
All	All	7067	0	6649	132	1

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 (132) 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:156[B]:MET:CE	1:B:163:PRO:HD3	1.97	0.94
1:B:156[B]:MET:HE3	1:B:163:PRO:HD3	1.50	0.93
1:A:1:MET:O	3:A:359:HOH:O	1.88	0.90
1:B:156[B]:MET:HE3	1:B:163:PRO:CD	2.02	0.88
1:C:8:LYS:NZ	3:C:426:HOH:O	2.07	0.88
1:A:135:LYS:HE3	1:A:160:GLU:OE1	1.84	0.78
1:A:24:VAL:O	1:A:54:TYR:OH	2.01	0.78
1:B:156[A]:MET:HE2	1:B:162:LYS:HE2	1.66	0.77
1:A:50:THR:HA	1:A:54:TYR:CE2	2.21	0.76
1:A:245:GLU:OE2	3:A:367:HOH:O	2.08	0.72
1:B:83:LYS:HG2	1:B:114:LEU:HB2	1.71	0.72
1:C:38:LYS:HD3	3:C:400:HOH:O	1.90	0.70
1:C:142:ILE:HD11	1:C:161:ILE:CD1	2.22	0.70
1:A:229:HIS:HB3	1:A:231:ILE:HD12	1.75	0.68
1:B:111:ASP:OD1	1:B:140[B]:LYS:HE3	1.92	0.68
1:B:140[B]:LYS:HB2	3:B:360:HOH:O	1.93	0.67
1:C:169:GLU:HG3	1:C:197[A]:MET:CE	2.25	0.67
1:C:169:GLU:HG3	1:C:197[A]:MET:HE3	1.77	0.67
1:A:150:HIS:HE1	1:A:276:ASP:OD1	1.77	0.67
1:C:142:ILE:HD11	1:C:161:ILE:HD12	1.80	0.64
1:B:156[B]:MET:HE3	1:B:163:PRO:HD2	1.80	0.63
1:B:156[B]:MET:HE1	1:B:163:PRO:HD3	1.79	0.63
1:B:177:LYS:HE3	3:B:344:HOH:O	1.98	0.63
1:B:156[A]:MET:HE2	1:B:162:LYS:CE	2.28	0.62
1:C:75:ARG:O	1:C:75:ARG:HD3	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:THR:HG22	3:C:366:HOH:O	2.01	0.61
1:C:177:LYS:HE3	3:C:420:HOH:O	2.01	0.61
1:B:5:LEU:HB3	1:B:6:GLN:HE21	1.65	0.60
1:C:91:TYR:HB2	1:C:125:GLU:HG3	1.83	0.60
1:C:177:LYS:CE	3:C:420:HOH:O	2.48	0.60
1:C:124:LYS:HE3	1:C:154:ASP:OD2	2.01	0.60
1:C:194:SER:O	1:C:197[A]:MET:HE2	2.02	0.59
1:B:150:HIS:HD2	3:B:305:HOH:O	1.85	0.58
1:B:156[A]:MET:HE2	1:B:162:LYS:CD	2.32	0.58
1:A:24:VAL:O	1:A:54:TYR:CZ	2.57	0.58
1:A:53:ILE:HG13	1:A:85:TRP:CE2	2.39	0.57
1:C:194:SER:HB2	1:C:197[A]:MET:CE	2.35	0.57
1:A:83:LYS:HE3	1:A:114:LEU:HD12	1.87	0.56
1:B:25:PHE:HB2	1:B:236[B]:LYS:HZ2	1.70	0.56
1:B:193[A]:TRP:CE3	1:B:236[A]:LYS:NZ	2.73	0.56
1:C:148:GLN:NE2	3:C:382:HOH:O	2.38	0.56
1:A:75:ARG:C	1:A:75:ARG:HD3	2.29	0.56
1:C:194:SER:HB2	1:C:197[A]:MET:HE2	1.87	0.56
1:A:24:VAL:HB	1:A:54:TYR:CE2	2.41	0.56
1:A:261:ARG:HD2	3:A:370:HOH:O	2.06	0.56
1:C:57:GLU:HG3	3:C:359:HOH:O	2.06	0.56
1:A:42:VAL:CG2	1:A:70:GLU:HG2	2.36	0.55
1:C:1:MET:HE3	1:C:19:TRP:HZ2	1.72	0.55
1:A:24:VAL:HB	1:A:54:TYR:HE2	1.71	0.54
1:B:25:PHE:HB2	1:B:236[B]:LYS:NZ	2.22	0.54
1:A:53:ILE:HG13	1:A:85:TRP:CD2	2.42	0.54
1:A:150:HIS:CE1	1:A:276:ASP:OD1	2.60	0.54
1:A:207:LEU:CD2	1:A:221:ILE:HD11	2.38	0.54
1:B:156[A]:MET:CE	1:B:162:LYS:HD3	2.37	0.54
1:B:194:SER:N	1:B:236[A]:LYS:HE2	2.23	0.53
1:A:30:GLY:O	1:A:31:SER:C	2.51	0.53
1:A:50:THR:HA	1:A:54:TYR:HE2	1.73	0.52
1:C:211:ALA:HB1	1:C:216:LYS:O	2.10	0.52
1:C:75:ARG:HD3	1:C:75:ARG:C	2.34	0.52
1:C:53:ILE:HD11	1:C:116:HIS:CE1	2.45	0.52
1:A:27:VAL:HG12	1:A:28:GLU:HA	1.92	0.52
1:B:234:ILE:O	1:B:236[A]:LYS:HD2	2.10	0.52
1:A:114:LEU:HD13	1:A:145[B]:SER:OG	2.10	0.51
1:A:237:SER:OG	1:A:242:ARG:HG2	2.10	0.51
1:B:156[A]:MET:HE2	1:B:162:LYS:HD3	1.92	0.51
1:A:50:THR:OG1	1:A:54:TYR:CD2	2.55	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:PRO:HD2	1:B:236[A]:LYS:HE2	1.94	0.50
1:B:236[A]:LYS:CD	1:B:236[A]:LYS:N	2.75	0.50
1:A:127:TRP:CH2	1:A:142:ILE:HG13	2.46	0.50
1:B:156[A]:MET:HE1	1:B:188:ILE:HD11	1.94	0.50
1:B:96:ALA:O	1:B:100:THR:HG23	2.12	0.49
1:C:202:LEU:HA	1:C:218:VAL:HG11	1.93	0.49
1:B:4:HIS:CD2	1:B:4:HIS:N	2.81	0.48
1:B:38:LYS:HD2	1:B:70:GLU:OE2	2.13	0.48
1:A:130:LEU:HD13	1:A:142:ILE:HG22	1.95	0.48
1:A:252:PHE:HE1	1:A:254:LEU:HD13	1.79	0.48
1:C:193[B]:TRP:HE3	3:C:423:HOH:O	1.95	0.48
1:A:236:LYS:O	1:A:237:SER:HB2	2.14	0.47
1:C:146:ASN:ND2	3:C:368:HOH:O	2.45	0.47
1:A:42:VAL:HG22	1:A:70:GLU:HG2	1.97	0.47
1:A:50:THR:CA	1:A:54:TYR:CE2	2.95	0.47
1:B:204:HIS:CE1	1:B:206:VAL:HG13	2.50	0.47
1:C:114:LEU:HD13	1:C:145[B]:SER:OG	2.15	0.46
1:A:242:ARG:HG3	1:A:242:ARG:HH11	1.79	0.46
1:A:207:LEU:HD22	1:A:221:ILE:HD11	1.97	0.46
1:B:60:VAL:HG22	1:B:105:LEU:CD2	2.46	0.46
1:B:160:GLU:HG2	1:B:161:ILE:HG13	1.98	0.46
1:C:38:LYS:HE2	1:C:70:GLU:OE2	2.16	0.45
1:C:252:PHE:HE1	1:C:254:LEU:HD13	1.81	0.45
1:A:42:VAL:HG21	1:A:70:GLU:HG2	1.98	0.45
1:C:177:LYS:HD3	1:C:181:ARG:NH2	2.32	0.45
1:A:29:GLU:OE2	1:A:56:ASN:HA	2.17	0.45
1:B:6:GLN:H	1:B:6:GLN:HG2	1.62	0.44
1:C:127:TRP:CG	1:C:155:LEU:HD11	2.53	0.44
1:C:258:ASP:O	1:C:262:ILE:HG13	2.18	0.44
1:A:113:TYR:HD2	1:A:130:LEU:HD22	1.81	0.44
1:B:129:ALA:O	1:B:132:THR:HG22	2.18	0.44
1:A:171:HIS:CE1	1:A:174:LEU:HB2	2.52	0.44
1:C:144:VAL:HG22	1:C:147:PHE:CE2	2.52	0.44
1:A:131:GLU:O	1:A:135:LYS:HD3	2.17	0.44
1:A:207:LEU:HD23	1:A:221:ILE:HD11	1.99	0.44
1:C:25:PHE:HB3	1:C:236[B]:LYS:HD3	1.99	0.44
1:A:93:GLU:HG2	3:A:368:HOH:O	2.18	0.43
1:B:144:VAL:HG22	1:B:147:PHE:CE2	2.53	0.43
1:A:5:LEU:HD13	1:A:44:GLY:C	2.42	0.43
1:A:212:GLN:HG3	1:A:213:THR:N	2.33	0.43
1:A:74:SER:HB3	1:A:76:GLU:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LYS:HD2	1:A:252:PHE:CD2	2.54	0.43
1:B:156[B]:MET:CE	1:B:163:PRO:CD	2.75	0.43
1:C:131:GLU:HG2	1:C:161:ILE:HG23	2.00	0.43
1:B:140[B]:LYS:HA	1:B:140[B]:LYS:HD2	1.50	0.42
1:B:144:VAL:HG13	1:B:147:PHE:HB2	2.01	0.42
1:A:84:VAL:HG23	1:A:115:ILE:HA	2.01	0.42
1:B:171:HIS:HB2	1:B:172:PRO:HD2	2.00	0.42
1:C:29:GLU:HA	1:C:33:LEU:HD12	2.01	0.42
1:B:99:GLU:OE2	1:B:138:ARG:NH2	2.37	0.42
1:B:95:LEU:HD21	1:B:132:THR:CG2	2.49	0.42
1:B:197:MET:O	1:B:200:GLN:HG3	2.20	0.41
1:C:169:GLU:HB2	1:C:193[A]:TRP:HZ3	1.84	0.41
1:A:25:PHE:CD1	1:A:236:LYS:HE3	2.55	0.41
1:B:171:HIS:HB2	1:B:172:PRO:CD	2.50	0.41
1:A:220:GLN:NE2	1:A:245:GLU:HG2	2.36	0.41
1:B:169:GLU:HB2	1:B:193[B]:TRP:CE3	2.56	0.41
1:A:24:VAL:HG12	1:A:25:PHE:H	1.86	0.41
1:C:169:GLU:HG3	1:C:197[A]:MET:HE1	1.98	0.41
1:A:32:GLU:CD	1:A:238:THR:HG21	2.47	0.40
1:C:127:TRP:CD1	1:C:155:LEU:HD11	2.55	0.40
1:B:5:LEU:HB3	1:B:6:GLN:NE2	2.34	0.40
1:B:27:VAL:HG23	1:B:33:LEU:HG	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LYS:NZ	3:B:333:HOH:O[2_455]	1.79	0.41

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	280/314 (89%)	266 (95%)	11 (4%)	3 (1%)	11	13
1	B	281/314 (90%)	273 (97%)	8 (3%)	0	100	100
1	C	283/314 (90%)	275 (97%)	8 (3%)	0	100	100
All	All	844/942 (90%)	814 (96%)	27 (3%)	3 (0%)	30	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	29	GLU
1	A	28	GLU

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	240/264 (91%)	203 (85%)	37 (15%)	2	3
1	B	241/264 (91%)	220 (91%)	21 (9%)	9	12
1	C	242/264 (92%)	211 (87%)	31 (13%)	4	4
All	All	723/792 (91%)	634 (88%)	89 (12%)	5	5

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	THR
1	A	5	LEU
1	A	8	LYS
1	A	26	GLN
1	A	28	GLU
1	A	33	LEU
1	A	48	ILE
1	A	53	ILE
1	A	69	GLU

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Mol	Chain	Res	Type
1	A	70	GLU
1	A	76	GLU
1	A	82	SER
1	A	84	VAL
1	A	110	LEU
1	A	120	GLU
1	A	128	ARG
1	A	130	LEU
1	A	135	LYS
1	A	142	ILE
1	A	144	VAL
1	A	160	GLU
1	A	168	VAL
1	A	174	LEU
1	A	176	GLN
1	A	198	GLN
1	A	200	GLN
1	A	212	GLN
1	A	213	THR
1	A	221	ILE
1	A	223	LEU
1	A	236	LYS
1	A	238	THR
1	A	249	VAL
1	A	254	LEU
1	A	256	GLN
1	A	269	LEU
1	B	4	HIS
1	B	6	GLN
1	B	22	LEU
1	B	33	LEU
1	B	60	VAL
1	B	70	GLU
1	B	93	GLU
1	B	100	THR
1	B	130	LEU
1	B	135	LYS
1	B	139	ILE
1	B	144	VAL
1	B	160	GLU
1	B	174	LEU
1	B	177	LYS

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Mol	Chain	Res	Type
1	B	206	VAL
1	B	223	LEU
1	B	236[A]	LYS
1	B	236[B]	LYS
1	B	254	LEU
1	B	269	LEU
1	C	1	MET
1	C	3	THR
1	C	8	LYS
1	C	10	THR
1	C	25	PHE
1	C	33	LEU
1	C	53	ILE
1	C	69	GLU
1	C	76	GLU
1	C	92	GLU
1	C	122	LYS
1	C	130	LEU
1	C	144	VAL
1	C	156	MET
1	C	157	THR
1	C	161	ILE
1	C	162	LYS
1	C	173	ARG
1	C	174	LEU
1	C	176	GLN
1	C	193[A]	TRP
1	C	193[B]	TRP
1	C	198	GLN
1	C	212	GLN
1	C	223	LEU
1	C	229	HIS
1	C	236[A]	LYS
1	C	236[B]	LYS
1	C	249	VAL
1	C	254	LEU
1	C	269	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN

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Mol	Chain	Res	Type
1	A	26	GLN
1	A	150	HIS
1	A	166	ASN
1	A	200	GLN
1	B	4	HIS
1	B	6	GLN
1	B	166	ASN
1	B	198	GLN
1	C	6	GLN
1	C	12	HIS
1	C	146	ASN
1	C	148	GLN
1	C	166	ASN
1	C	176	GLN
1	C	189	GLN
1	C	215	ASN
1	C	229	HIS
1	C	241	HIS
1	C	256	GLN

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 ⓘ

Of 4 ligands modelled in this entry, 4 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	280/314 (89%)	0.09	9 (3%)	50	52	5, 24, 36, 49	5 (1%)
1	B	277/314 (88%)	0.07	5 (1%)	67	69	10, 24, 34, 46	6 (2%)
1	C	280/314 (89%)	0.13	3 (1%)	78	79	12, 24, 32, 41	5 (1%)
All	All	837/942 (88%)	0.10	17 (2%)	65	66	5, 24, 34, 49	16 (1%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	GLU	11.9
1	A	54	TYR	7.6
1	A	25	PHE	5.3
1	A	26	GLN	4.7
1	A	193	TRP	4.5
1	C	1	MET	3.7
1	A	29	GLU	3.4
1	C	193[A]	TRP	3.3
1	C	279	ASP	3.2
1	B	4	HIS	2.6
1	A	120	GLU	2.5
1	A	279	ASP	2.2
1	B	193[A]	TRP	2.2
1	A	280	PHE	2.2
1	B	280	PHE	2.2
1	B	242	ARG	2.1
1	B	6	GLN	2.1

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	CA	A	282	1/1	0.85	0.10	51,51,51,51	0
2	CA	B	281	1/1	0.97	0.18	31,31,31,31	0
2	CA	C	281	1/1	0.97	0.21	25,25,25,25	0
2	CA	A	281	1/1	0.98	0.15	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.