



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:55 AM UTC

PDB ID : 3O06 / pdb_00003o06
Title : Crystal Structure of yeast pyridoxal 5-phosphate synthase Snz1
Authors : Teng, Y.B.; Zhang, X.; Zhou, C.Z.; Hu, H.X.
Deposited on : 2010-07-19
Resolution : 2.35 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

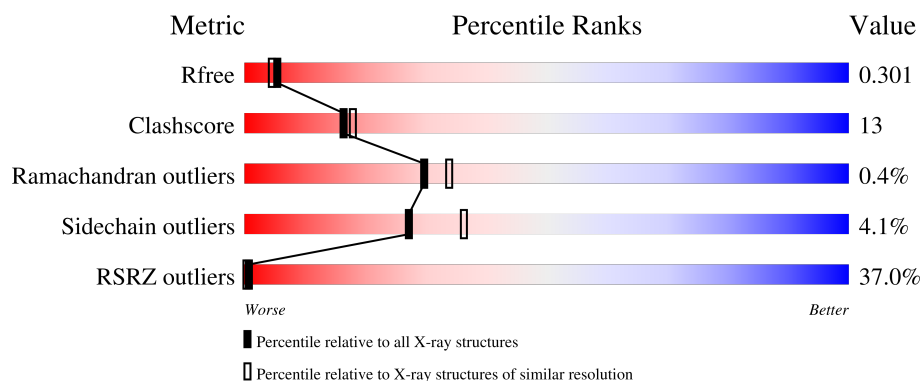
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	291	11% 68% 19% • 11%
1	B	291	10% 73% 12% • • 11%
1	C	291	77% 71% 15% • 11%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 5875 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 Pyridoxine biosynthesis protein SNZ1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			1933	1214	331	373	15			
1	B	258	Total	C	N	O	S	0	0	0
			1933	1214	331	373	15			
1	C	258	Total	C	N	O	S	0	0	0
			1933	1214	331	373	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	expression tag	UNP Q03148
A	8	HIS	-	expression tag	UNP Q03148
A	9	HIS	-	expression tag	UNP Q03148
A	10	HIS	-	expression tag	UNP Q03148
A	11	HIS	-	expression tag	UNP Q03148
A	12	HIS	-	expression tag	UNP Q03148
A	13	HIS	-	expression tag	UNP Q03148
A	14	GLY	-	expression tag	UNP Q03148
B	7	MET	-	expression tag	UNP Q03148
B	8	HIS	-	expression tag	UNP Q03148
B	9	HIS	-	expression tag	UNP Q03148
B	10	HIS	-	expression tag	UNP Q03148
B	11	HIS	-	expression tag	UNP Q03148
B	12	HIS	-	expression tag	UNP Q03148
B	13	HIS	-	expression tag	UNP Q03148
B	14	GLY	-	expression tag	UNP Q03148
C	7	MET	-	expression tag	UNP Q03148
C	8	HIS	-	expression tag	UNP Q03148
C	9	HIS	-	expression tag	UNP Q03148
C	10	HIS	-	expression tag	UNP Q03148
C	11	HIS	-	expression tag	UNP Q03148
C	12	HIS	-	expression tag	UNP Q03148
C	13	HIS	-	expression tag	UNP Q03148

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Chain	Residue	Modelled	Actual	Comment	Reference
C	14	GLY	-	expression tag	UNP Q03148

- Molecule 2 is water.

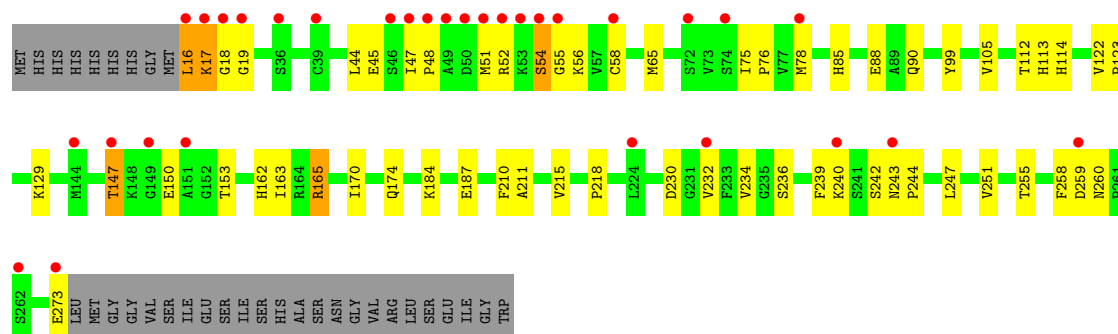
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	29	Total	O	0	0
			29	29		
2	B	20	Total	O	0	0
			20	20		
2	C	27	Total	O	0	0
			27	27		

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.

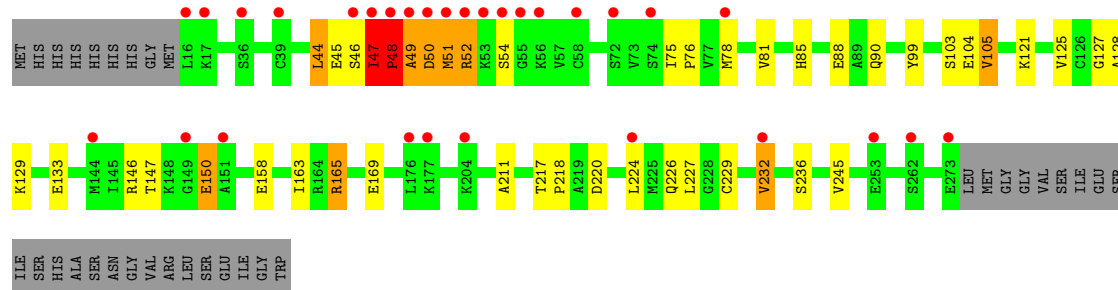
• Molecule 1: Pyridoxine biosynthesis protein SNZ1

Chain A: 



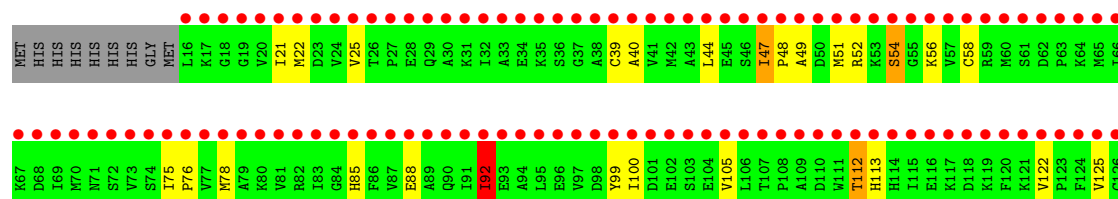
• Molecule 1: Pyridoxine biosynthesis protein SNZ1

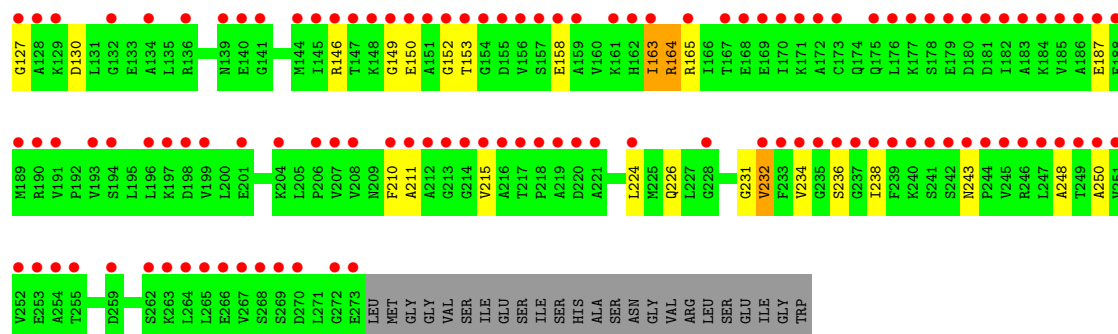
Chain B: 



• Molecule 1: Pyridoxine biosynthesis protein SNZ1

Chain C: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	59.31Å 110.38Å 156.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	110.38 – 2.35 90.18 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.5 (110.38-2.35) 99.5 (90.18-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.22 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.204 , 0.251 0.271 , 0.301	Depositor DCC
R_{free} test set	2175 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5875	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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	1.29	4/1958 (0.2%)	1.16	1/2640 (0.0%)
1	B	1.20	3/1958 (0.2%)	1.12	4/2640 (0.2%)
1	C	1.26	4/1958 (0.2%)	1.16	6/2640 (0.2%)
All	All	1.25	11/5874 (0.2%)	1.15	11/7920 (0.1%)

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	B	0	2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	GLY	C-N	-6.75	1.24	1.33
1	B	81	VAL	C-O	6.03	1.30	1.23
1	A	260	ASN	C-O	-5.99	1.18	1.24
1	A	165	ARG	C-O	-5.91	1.17	1.24
1	A	258	PHE	C-O	-5.82	1.16	1.24
1	B	165	ARG	C-O	-5.70	1.17	1.24
1	B	44	LEU	C-O	-5.63	1.16	1.23
1	C	92	ILE	CA-CB	5.56	1.60	1.54
1	C	164	ARG	C-O	-5.51	1.17	1.24
1	C	231	GLY	N-CA	5.21	1.50	1.45
1	C	250	ALA	CA-C	5.01	1.59	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	THR	CB-CA-C	8.60	127.30	109.68
1	B	48	PRO	CA-C-N	6.88	134.67	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	48	PRO	C-N-CA	6.88	134.67	121.54
1	C	152	GLY	N-CA-C	6.71	123.07	115.08
1	C	243	ASN	CA-C-N	6.32	126.06	119.05
1	C	243	ASN	C-N-CA	6.32	126.06	119.05
1	C	232	VAL	N-CA-C	6.13	116.45	108.35
1	C	75	ILE	CA-C-N	6.12	126.08	119.78
1	C	75	ILE	C-N-CA	6.12	126.08	119.78
1	B	245	VAL	CB-CA-C	-5.61	104.48	112.22
1	B	150	GLU	N-CA-C	-5.07	98.40	107.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	47	ILE	Peptide,Mainchain

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	1933	0	1989	50	0
1	B	1933	0	1989	54	0
1	C	1933	0	1989	52	0
2	A	29	0	0	1	0
2	B	20	0	0	0	0
2	C	27	0	0	0	0
All	All	5875	0	5967	153	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 13.

All (153) 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:C:47:ILE:CD1	1:C:236:SER:HB2	1.60	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:PRO:HG2	1:B:105:VAL:CG1	1.71	1.21
1:C:47:ILE:HD12	1:C:236:SER:CB	1.72	1.17
1:B:48:PRO:CG	1:B:105:VAL:HG12	1.74	1.16
1:B:211:ALA:HB3	1:B:232:VAL:HG22	1.22	1.09
1:C:47:ILE:HD12	1:C:236:SER:HB2	1.21	1.08
1:C:47:ILE:CD1	1:C:236:SER:CB	2.30	1.04
1:C:48:PRO:HG2	1:C:105:VAL:HG12	1.38	1.01
1:B:48:PRO:HG2	1:B:105:VAL:HG12	1.32	1.01
1:B:48:PRO:CG	1:B:105:VAL:CG1	2.38	0.99
1:B:47:ILE:HG21	1:B:236:SER:OG	1.64	0.97
1:C:48:PRO:HG2	1:C:105:VAL:CG1	1.96	0.94
1:A:17:LYS:HE3	1:A:17:LYS:H	1.32	0.91
1:A:16:LEU:HB3	1:A:99:TYR:OH	1.72	0.90
1:C:149:GLY:HA2	1:C:158:GLU:HB3	1.53	0.90
1:B:211:ALA:HB3	1:B:232:VAL:CG2	2.03	0.89
1:A:147:THR:HG23	1:A:162:HIS:HB2	1.57	0.87
1:B:48:PRO:HG3	1:B:105:VAL:HG12	1.56	0.86
1:A:16:LEU:N	1:A:16:LEU:HD23	1.91	0.86
1:B:48:PRO:HG2	1:B:105:VAL:HG11	1.59	0.83
1:A:242:SER:OG	1:A:273:GLU:HB3	1.78	0.82
1:B:47:ILE:CG2	1:B:236:SER:OG	2.26	0.82
1:A:19:GLY:O	1:A:255:THR:HG21	1.81	0.81
1:C:47:ILE:HD12	1:C:236:SER:OG	1.80	0.81
1:A:54:SER:HB2	1:A:56:LYS:HG2	1.64	0.80
1:B:103:SER:OG	1:B:105:VAL:HG23	1.83	0.78
1:B:47:ILE:O	1:B:48:PRO:C	2.30	0.73
1:A:211:ALA:HB3	1:A:232:VAL:HG22	1.69	0.73
1:C:47:ILE:HD11	1:C:236:SER:H	1.55	0.72
1:C:47:ILE:HD11	1:C:236:SER:CB	2.20	0.71
1:B:163:ILE:CD1	1:B:227:LEU:HB3	2.21	0.70
1:C:78:MET:HG2	1:C:99:TYR:HB2	1.72	0.69
1:A:147:THR:CG2	1:A:162:HIS:HB2	2.22	0.68
1:A:47:ILE:HD13	1:A:240:LYS:NZ	2.08	0.68
1:B:47:ILE:O	1:B:49:ALA:N	2.26	0.68
1:A:90:GLN:HE22	1:B:226:GLN:HE22	1.40	0.67
1:B:47:ILE:HG21	1:B:236:SER:CB	2.25	0.67
1:B:90:GLN:HE22	1:C:226:GLN:HE22	1.42	0.67
1:B:49:ALA:O	1:B:52:ARG:N	2.28	0.66
1:C:211:ALA:CB	1:C:224:LEU:HD13	2.26	0.65
1:C:215:VAL:HG11	1:C:232:VAL:HG11	1.79	0.65
1:A:147:THR:HG23	1:A:162:HIS:CB	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ILE:HD11	1:B:227:LEU:HB3	1.79	0.64
1:A:17:LYS:O	1:A:210:PHE:CZ	2.51	0.64
1:B:49:ALA:O	1:B:51:MET:N	2.30	0.64
1:B:165:ARG:NE	1:B:169:GLU:OE2	2.30	0.64
1:A:47:ILE:HD13	1:A:240:LYS:HZ1	1.61	0.64
1:C:47:ILE:HD11	1:C:236:SER:HB2	1.73	0.64
1:A:17:LYS:HE3	1:A:17:LYS:N	2.10	0.64
1:C:51:MET:HE3	1:C:58:CYS:SG	2.39	0.63
1:C:47:ILE:CD1	1:C:236:SER:OG	2.41	0.63
1:C:150:GLU:OE2	1:C:153:THR:HG21	1.97	0.63
1:A:16:LEU:N	1:A:17:LYS:HE3	2.13	0.62
1:A:85:HIS:CD2	1:A:88:GLU:H	2.18	0.62
1:A:112:THR:HB	1:A:113:HIS:HD2	1.63	0.62
1:B:165:ARG:NH2	1:B:169:GLU:OE2	2.33	0.62
1:B:211:ALA:HB1	1:B:224:LEU:HD13	1.82	0.61
1:A:16:LEU:N	1:A:16:LEU:CD2	2.63	0.61
1:A:112:THR:HB	1:A:113:HIS:CD2	2.35	0.61
1:B:163:ILE:HD11	1:B:227:LEU:CB	2.31	0.60
1:A:54:SER:HB2	1:A:56:LYS:CG	2.33	0.58
1:B:44:LEU:N	1:B:44:LEU:HD23	2.19	0.58
1:C:44:LEU:HD12	1:C:44:LEU:O	2.05	0.57
1:C:48:PRO:CG	1:C:105:VAL:HG12	2.25	0.57
1:C:48:PRO:CG	1:C:105:VAL:CG1	2.78	0.57
1:C:47:ILE:HG22	1:C:49:ALA:H	1.69	0.57
1:C:211:ALA:HB1	1:C:224:LEU:HD13	1.86	0.57
1:B:163:ILE:HD11	1:B:227:LEU:HD13	1.85	0.56
1:A:170:ILE:O	1:A:174:GLN:HG3	2.06	0.56
1:B:48:PRO:CG	1:B:105:VAL:HG11	2.25	0.56
1:C:100:ILE:HD12	1:C:122:VAL:HG11	1.85	0.56
1:C:130:ASP:HB3	1:C:165:ARG:HD3	1.87	0.56
1:B:47:ILE:O	1:B:47:ILE:HG12	2.07	0.55
1:C:85:HIS:CD2	1:C:88:GLU:H	2.23	0.55
1:B:49:ALA:C	1:B:51:MET:N	2.64	0.55
1:A:17:LYS:O	1:A:210:PHE:CE2	2.60	0.55
1:C:112:THR:HB	1:C:113:HIS:CD2	2.42	0.55
1:C:92:ILE:HG21	1:C:100:ILE:HG12	1.88	0.54
1:C:47:ILE:HD13	1:C:236:SER:HB2	1.78	0.54
1:A:51:MET:HE3	1:A:58:CYS:SG	2.48	0.53
1:B:165:ARG:CZ	1:B:169:GLU:OE2	2.57	0.53
1:A:85:HIS:CD2	1:A:88:GLU:HG3	2.43	0.53
1:C:48:PRO:HB2	1:C:105:VAL:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:PRO:HG2	1:A:105:VAL:HG11	1.91	0.53
1:C:51:MET:O	1:C:54:SER:N	2.42	0.53
1:A:112:THR:O	1:A:112:THR:HG22	2.08	0.52
1:A:150:GLU:OE2	1:A:153:THR:HG21	2.10	0.52
1:A:17:LYS:H	1:A:17:LYS:CE	2.13	0.52
1:B:85:HIS:CD2	1:B:88:GLU:H	2.27	0.52
1:C:21:ILE:HG12	1:C:40:ALA:HB3	1.93	0.51
1:A:16:LEU:HB3	1:A:99:TYR:HH	1.74	0.51
1:A:150:GLU:CD	1:A:153:THR:HG21	2.35	0.51
1:B:78:MET:HG2	1:B:99:TYR:HB2	1.92	0.50
1:A:247:LEU:O	1:A:251:VAL:HG23	2.11	0.50
1:A:17:LYS:O	1:A:210:PHE:HZ	1.94	0.50
1:C:215:VAL:HG21	1:C:232:VAL:CG1	2.42	0.50
1:A:242:SER:HG	1:A:273:GLU:HB3	1.75	0.49
1:C:47:ILE:CG2	1:C:49:ALA:HB3	2.41	0.49
1:C:149:GLY:HA2	1:C:158:GLU:CB	2.33	0.49
1:A:85:HIS:HD2	1:A:88:GLU:H	1.57	0.49
1:C:149:GLY:CA	1:C:158:GLU:HB3	2.35	0.49
1:A:45:GLU:HA	1:A:65:MET:HE3	1.95	0.49
1:B:50:ASP:O	1:B:54:SER:OG	2.23	0.49
1:A:114:HIS:HE1	2:A:317:HOH:O	1.96	0.48
1:A:122:VAL:HG23	1:A:123:PRO:HD2	1.95	0.48
1:B:163:ILE:CD1	1:B:227:LEU:CB	2.91	0.48
1:B:49:ALA:O	1:B:50:ASP:C	2.56	0.48
1:A:215:VAL:HG11	1:A:232:VAL:HG11	1.96	0.47
1:A:47:ILE:HG12	1:A:236:SER:CB	2.45	0.47
1:B:147:THR:HG21	1:B:163:ILE:HG23	1.96	0.46
1:C:100:ILE:CD1	1:C:122:VAL:HG11	2.45	0.46
1:C:163:ILE:HG23	1:C:164:ARG:N	2.31	0.46
1:A:129:LYS:HB2	1:A:162:HIS:CD2	2.51	0.46
1:C:146:ARG:HA	1:C:210:PHE:O	2.15	0.46
1:C:238:ILE:HG21	1:C:248:ALA:HB2	1.97	0.46
1:A:85:HIS:HE1	1:B:220:ASP:OD1	1.98	0.46
1:B:44:LEU:HG	1:B:46:SER:O	2.16	0.46
1:B:49:ALA:C	1:B:51:MET:H	2.23	0.46
1:A:78:MET:HG2	1:A:99:TYR:HB2	1.99	0.45
1:C:100:ILE:HD12	1:C:122:VAL:CG1	2.45	0.45
1:B:129:LYS:N	1:B:133:GLU:OE1	2.47	0.45
1:B:44:LEU:N	1:B:44:LEU:CD2	2.80	0.44
1:A:17:LYS:HB2	1:A:18:GLY:H	1.50	0.44
1:B:150:GLU:HB2	1:B:158:GLU:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:PRO:HG3	1:B:105:VAL:CG1	2.24	0.43
1:A:234:VAL:HG11	1:A:251:VAL:HG11	1.99	0.43
1:C:211:ALA:HB3	1:C:232:VAL:HG22	2.01	0.43
1:A:243:ASN:HA	1:A:244:PRO:HD3	1.76	0.43
1:B:163:ILE:HG21	1:B:229:CYS:SG	2.58	0.43
1:A:44:LEU:HD23	1:A:44:LEU:HA	1.68	0.43
1:B:163:ILE:HD11	1:B:227:LEU:CD1	2.48	0.43
1:C:25:VAL:HG12	1:C:44:LEU:HD12	2.00	0.43
1:C:47:ILE:C	1:C:49:ALA:H	2.27	0.43
1:B:128:ALA:HA	1:B:133:GLU:OE1	2.19	0.43
1:C:22:MET:HG2	1:C:234:VAL:CG2	2.49	0.43
1:A:75:ILE:HB	1:A:76:PRO:CD	2.49	0.42
1:C:215:VAL:HG21	1:C:232:VAL:HG13	2.01	0.42
1:C:39:CYS:O	1:C:76:PRO:HD2	2.20	0.42
1:B:75:ILE:HB	1:B:76:PRO:HD2	2.00	0.42
1:B:103:SER:HG	1:B:105:VAL:HG23	1.83	0.42
1:B:127:GLY:HA2	1:B:146:ARG:O	2.20	0.42
1:C:92:ILE:CG2	1:C:100:ILE:HG12	2.49	0.42
1:B:78:MET:HE2	1:B:99:TYR:CG	2.55	0.42
1:C:78:MET:HE2	1:C:99:TYR:CG	2.54	0.41
1:C:92:ILE:HD13	1:C:92:ILE:HA	1.77	0.41
1:A:236:SER:O	1:A:239:PHE:N	2.51	0.41
1:B:48:PRO:HB2	1:B:49:ALA:H	1.61	0.41
1:B:217:THR:HB	1:B:218:PRO:HD2	2.02	0.41
1:C:127:GLY:HA2	1:C:146:ARG:O	2.20	0.41
1:B:104:GLU:H	1:B:104:GLU:CD	2.28	0.40
1:C:47:ILE:HD11	1:C:236:SER:N	2.30	0.40
1:A:18:GLY:CA	1:A:230:ASP:O	2.70	0.40
1:B:121:LYS:HA	1:B:121:LYS:HD2	1.90	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	256/291 (88%)	243 (95%)	13 (5%)	0	100	100
1	B	256/291 (88%)	245 (96%)	8 (3%)	3 (1%)	10	9
1	C	256/291 (88%)	249 (97%)	7 (3%)	0	100	100
All	All	768/873 (88%)	737 (96%)	28 (4%)	3 (0%)	30	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	48	PRO
1	B	49	ALA
1	B	50	ASP

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	211/238 (89%)	201 (95%)	10 (5%)	23	30
1	B	211/238 (89%)	204 (97%)	7 (3%)	33	44
1	C	211/238 (89%)	202 (96%)	9 (4%)	26	34
All	All	633/714 (89%)	607 (96%)	26 (4%)	27	36

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	17	LYS
1	A	52	ARG
1	A	54	SER
1	A	163	ILE
1	A	165	ARG
1	A	184	LYS
1	A	187	GLU
1	A	218	PRO
1	A	259	ASP

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Mol	Chain	Res	Type
1	B	45	GLU
1	B	47	ILE
1	B	51	MET
1	B	52	ARG
1	B	105	VAL
1	B	125	VAL
1	B	232	VAL
1	C	47	ILE
1	C	52	ARG
1	C	54	SER
1	C	56	LYS
1	C	92	ILE
1	C	112	THR
1	C	125	VAL
1	C	163	ILE
1	C	187	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	A	113	HIS
1	A	114	HIS
1	A	139	ASN
1	A	174	GLN
1	A	226	GLN
1	B	85	HIS
1	B	113	HIS
1	B	114	HIS
1	B	139	ASN
1	B	162	HIS
1	B	175	GLN
1	B	226	GLN
1	C	85	HIS
1	C	113	HIS
1	C	114	HIS
1	C	226	GLN

5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	258/291 (88%)	0.62	31 (12%) 9 10	5, 25, 57, 99	15 (5%)
1	B	258/291 (88%)	0.80	30 (11%) 9 11	4, 27, 60, 99	15 (5%)
1	C	258/291 (88%)	4.16	225 (87%) 0 0	15, 59, 96, 123	15 (5%)
All	All	774/873 (88%)	1.86	286 (36%) 1 0	4, 34, 87, 123	45 (5%)

All (286) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	58	CYS	14.0
1	C	47	ILE	13.6
1	B	48	PRO	12.6
1	C	49	ALA	12.3
1	C	51	MET	11.9
1	B	47	ILE	11.6
1	C	39	CYS	11.5
1	C	48	PRO	11.5
1	C	46	SER	10.9
1	C	36	SER	10.6
1	C	72	SER	9.2
1	B	49	ALA	9.2
1	C	44	LEU	8.8
1	C	78	MET	8.8
1	C	52	ARG	8.7
1	C	224	LEU	8.6
1	C	74	SER	8.5
1	A	51	MET	8.4
1	B	39	CYS	8.1
1	C	43	ALA	8.1
1	C	262	SER	8.0
1	B	36	SER	8.0
1	B	46	SER	7.9

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Mol	Chain	Res	Type	RSRZ
1	C	150	GLU	7.8
1	A	262	SER	7.8
1	C	238	ILE	7.7
1	A	47	ILE	7.7
1	C	50	ASP	7.7
1	C	45	GLU	7.7
1	C	149	GLY	7.6
1	C	55	GLY	7.5
1	C	57	VAL	7.5
1	A	48	PRO	7.4
1	B	51	MET	7.4
1	A	74	SER	7.3
1	A	49	ALA	7.3
1	C	56	LYS	7.2
1	C	111	TRP	7.2
1	C	144	MET	7.0
1	C	240	LYS	7.0
1	C	68	ASP	6.8
1	A	39	CYS	6.7
1	C	239	PHE	6.7
1	B	58	CYS	6.7
1	C	62	ASP	6.7
1	C	59	ARG	6.5
1	C	92	ILE	6.5
1	C	18	GLY	6.5
1	B	74	SER	6.4
1	C	65	MET	6.4
1	B	262	SER	6.4
1	C	24	VAL	6.4
1	B	72	SER	6.3
1	C	61	SER	6.3
1	C	32	ILE	6.3
1	C	242	SER	6.2
1	C	27	PRO	6.2
1	C	151	ALA	6.2
1	C	66	ILE	6.1
1	C	245	VAL	6.1
1	C	69	ILE	6.0
1	C	73	VAL	6.0
1	A	36	SER	6.0
1	A	58	CYS	5.9
1	C	25	VAL	5.9

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Mol	Chain	Res	Type	RSRZ
1	C	232	VAL	5.9
1	A	224	LEU	5.8
1	C	241	SER	5.8
1	C	270	ASP	5.7
1	B	224	LEU	5.7
1	C	53	LYS	5.6
1	C	71	ASN	5.6
1	C	67	LYS	5.5
1	C	109	ALA	5.5
1	B	52	ARG	5.5
1	C	35	LYS	5.5
1	A	16	LEU	5.4
1	C	60	MET	5.4
1	C	97	VAL	5.4
1	A	72	SER	5.3
1	C	235	GLY	5.3
1	C	89	ALA	5.3
1	C	105	VAL	5.3
1	C	30	ALA	5.2
1	A	19	GLY	5.2
1	B	50	ASP	5.2
1	C	94	ALA	5.1
1	C	236	SER	5.1
1	C	91	ILE	5.1
1	C	81	VAL	5.1
1	C	244	PRO	5.0
1	C	106	LEU	5.0
1	C	147	THR	4.9
1	A	52	ARG	4.9
1	C	33	ALA	4.9
1	C	177	LYS	4.9
1	C	17	LYS	4.8
1	C	100	ILE	4.8
1	A	50	ASP	4.8
1	C	19	GLY	4.8
1	C	54	SER	4.8
1	C	31	LYS	4.8
1	C	273	GLU	4.8
1	C	108	PRO	4.7
1	C	64	LYS	4.7
1	C	99	TYR	4.7
1	C	243	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	176	LEU	4.6
1	C	82	ARG	4.6
1	C	107	THR	4.6
1	C	95	LEU	4.6
1	A	18	GLY	4.6
1	C	148	LYS	4.6
1	C	23	ASP	4.6
1	C	87	VAL	4.6
1	A	78	MET	4.6
1	B	144	MET	4.6
1	C	122	VAL	4.6
1	C	248	ALA	4.5
1	C	185	VAL	4.5
1	B	53	LYS	4.5
1	C	121	LYS	4.5
1	C	212	ALA	4.4
1	C	80	LYS	4.4
1	B	54	SER	4.4
1	C	85	HIS	4.4
1	C	120	PHE	4.4
1	C	88	GLU	4.3
1	B	273	GLU	4.3
1	B	78	MET	4.3
1	C	182	ILE	4.3
1	A	17	LYS	4.3
1	C	79	ALA	4.2
1	C	250	ALA	4.2
1	C	41	VAL	4.2
1	C	175	GLN	4.2
1	C	213	GLY	4.2
1	A	144	MET	4.2
1	C	26	THR	4.2
1	C	237	GLY	4.1
1	C	119	LYS	4.1
1	C	112	THR	4.1
1	C	103	SER	4.1
1	C	181	ASP	4.1
1	A	53	LYS	4.1
1	C	40	ALA	4.1
1	C	180	ASP	4.1
1	C	34	GLU	4.1
1	C	76	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	193	VAL	4.1
1	C	42	MET	4.0
1	C	75	ILE	4.0
1	C	173	CYS	4.0
1	C	86	PHE	4.0
1	A	46	SER	4.0
1	C	114	HIS	4.0
1	C	90	GLN	4.0
1	C	156	VAL	3.9
1	C	247	LEU	3.9
1	C	110	ASP	3.9
1	C	234	VAL	3.9
1	C	128	ALA	3.9
1	C	118	ASP	3.8
1	B	149	GLY	3.8
1	C	84	GLY	3.8
1	C	165	ARG	3.8
1	A	54	SER	3.8
1	C	63	PRO	3.8
1	C	217	THR	3.8
1	C	22	MET	3.8
1	C	189	MET	3.8
1	C	124	PHE	3.8
1	C	154	GLY	3.8
1	C	83	ILE	3.7
1	C	215	VAL	3.7
1	C	28	GLU	3.7
1	C	253	GLU	3.7
1	C	172	ALA	3.7
1	C	216	ALA	3.7
1	A	273	GLU	3.7
1	C	246	ARG	3.7
1	B	55	GLY	3.7
1	C	179	GLU	3.7
1	C	187	GLU	3.7
1	C	20	VAL	3.7
1	C	252	VAL	3.7
1	C	194	SER	3.7
1	C	267	VAL	3.6
1	C	269	SER	3.6
1	A	55	GLY	3.6
1	A	243	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	21	ILE	3.6
1	C	198	ASP	3.6
1	C	146	ARG	3.5
1	C	37	GLY	3.5
1	C	132	GLY	3.5
1	C	259	ASP	3.5
1	C	214	GLY	3.5
1	C	129	LYS	3.5
1	C	16	LEU	3.5
1	C	233	PHE	3.5
1	C	77	VAL	3.4
1	C	251	VAL	3.4
1	A	149	GLY	3.4
1	C	29	GLN	3.4
1	C	249	THR	3.4
1	C	191	VAL	3.4
1	C	266	GLU	3.4
1	C	101	ASP	3.3
1	B	151	ALA	3.3
1	C	104	GLU	3.3
1	C	153	THR	3.3
1	C	183	ALA	3.2
1	A	232	VAL	3.1
1	A	259	ASP	3.1
1	C	218	PRO	3.1
1	C	125	VAL	3.1
1	C	158	GLU	3.1
1	C	38	ALA	3.1
1	C	152	GLY	3.0
1	C	197	LYS	3.0
1	C	184	LYS	3.0
1	C	126	CYS	3.0
1	C	162	HIS	3.0
1	C	190	ARG	2.9
1	C	188	GLU	2.9
1	C	98	ASP	2.9
1	C	265	LEU	2.9
1	C	93	GLU	2.9
1	C	70	MET	2.8
1	C	263	LYS	2.8
1	C	155	ASP	2.8
1	C	127	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	211	ALA	2.8
1	C	115	ILE	2.8
1	C	220	ASP	2.8
1	C	141	GLY	2.8
1	C	221	ALA	2.8
1	C	171	LYS	2.7
1	C	116	GLU	2.7
1	B	232	VAL	2.7
1	B	17	LYS	2.7
1	C	163	ILE	2.7
1	A	151	ALA	2.6
1	C	145	ILE	2.6
1	C	113	HIS	2.5
1	C	96	GLU	2.5
1	C	161	LYS	2.5
1	C	208	VAL	2.5
1	C	196	LEU	2.5
1	C	272	GLY	2.5
1	C	264	LEU	2.4
1	C	219	ALA	2.4
1	C	254	ALA	2.4
1	B	204	LYS	2.4
1	C	169	GLU	2.4
1	C	102	GLU	2.4
1	C	206	PRO	2.4
1	B	176	LEU	2.4
1	C	201	GLU	2.4
1	B	56	LYS	2.3
1	B	177	LYS	2.3
1	C	186	ALA	2.3
1	C	199	VAL	2.3
1	C	210	PHE	2.3
1	C	168	GLU	2.3
1	C	159	ALA	2.3
1	A	147	THR	2.3
1	C	268	SER	2.3
1	C	134	ALA	2.3
1	C	123	PRO	2.2
1	C	140	GLU	2.2
1	C	167	THR	2.2
1	C	157	SER	2.2
1	C	178	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	139	ASN	2.2
1	A	240	LYS	2.2
1	C	255	THR	2.1
1	C	136	ARG	2.1
1	B	16	LEU	2.1
1	C	117	LYS	2.1
1	C	207	VAL	2.1
1	C	170	ILE	2.0
1	C	228	GLY	2.0
1	B	253	GLU	2.0
1	C	204	LYS	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.