



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:29 PM UTC

PDB ID : 1YBF / pdb_00001ybf
Title : Crystal structure of AMP nucleosidase from Bacteroides thetaiotaomicron VPI-5482
Authors : Krishnamurthy, N.R.; Swaminathan, S.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2004-12-20
Resolution : 2.90 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

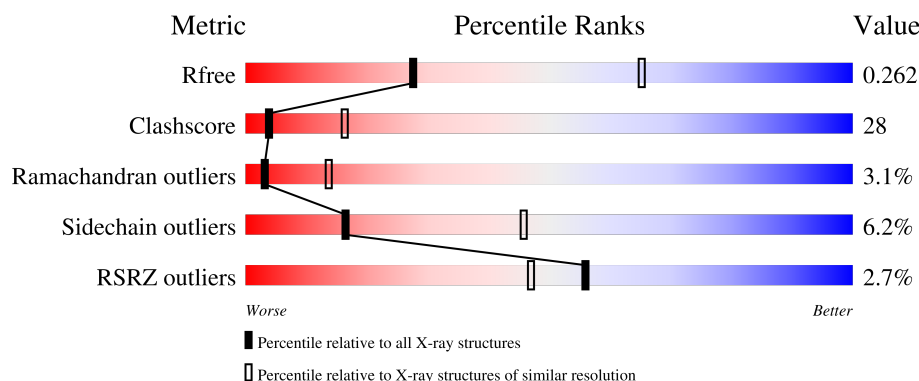
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	268	
1	B	268	
1	C	268	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5471 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 AMP nucleosidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	Se	0	0	0
			1876	1205	308	354	1	8			
1	B	228	Total	C	N	O	S	Se	0	0	0
			1778	1142	294	334	1	7			
1	C	230	Total	C	N	O	S	Se	0	0	0
			1801	1161	295	336	1	8			

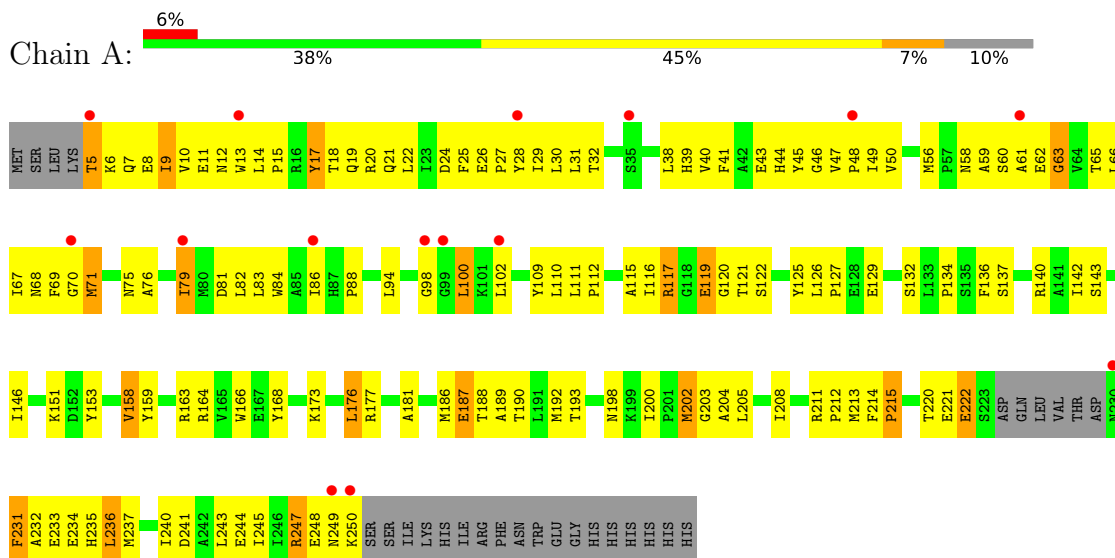
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	O	0	0
			3	3		
2	B	3	Total	O	0	0
			3	3		
2	C	10	Total	O	0	0
			10	10		

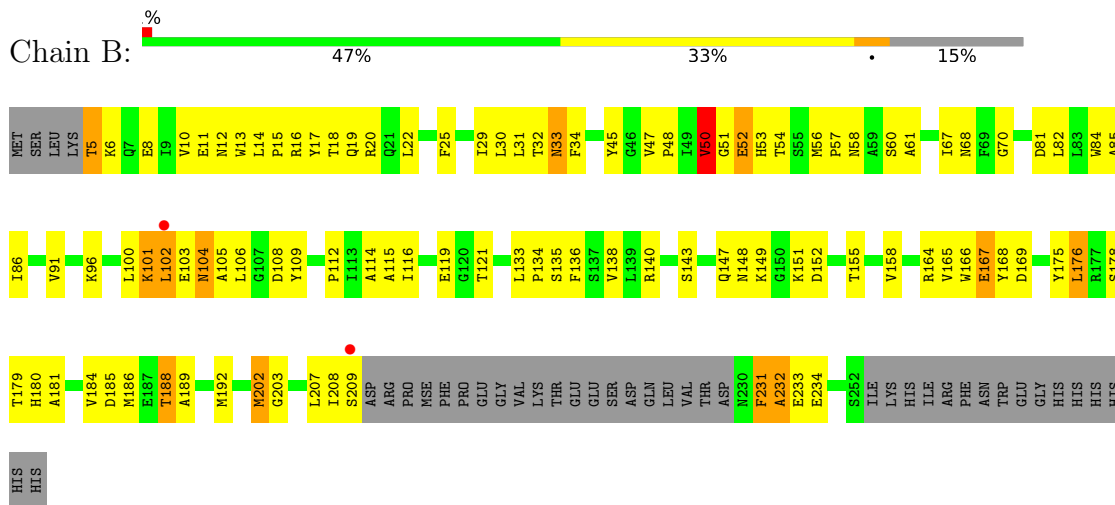
3 Residue-property plots [i](#)

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: AMP nucleosidase



• Molecule 1: AMP nucleosidase



• Molecule 1: AMP nucleosidase



MET	M80	D174	SER
SER	D81	Y175	SER
LEU	L82	L176	ILE
K4	L83	R177	LYS
T5	W84	S178	HIS
K6	A85	T179	ILE
Q7		H180	ARG
E8	P88	A181	PHE
I9		S182	ASN
V10	V91	G183	TRP
E11	I92	V184	GLU
N12		D185	GLY
W13	K86	M186	HIS
L14		E187	HIS
P15	L100	T188	HIS
R16	LYS	A189	HIS
R17	LEU	T190	HIS
T18	GLU	L191	HIS
Q19	ASN	M192	HIS
R20	A105		
Q21	L106	G195	
L22	G107	I200	
	D108	P201	
F25		M202	
E26	I116		
	R117	R211	
I29	G118	P212	
	E119	M213	
T32		M214	
N33	N123	P215	
F34		E216	
S35	E128	GLY	
H36		VAL	
Y37	L133	LYS	
L38		THR	
H39	R140	GLU	
V40	A141	GLU	
	I142	SER	
V47	S143	ASP	
	S144	GLN	
V50	A145	LEU	
	I146	VAL	
T54	Q147	THR	
S55	N148	ASP	
M56	K149	M230	
	G150	F231	
A61		A232	
E62	Y153	E233	
G63	W154		
	T155	M237	
L66			
I67	R163	D241	
N68		A242	
	E167	L243	
M71	Y168		
G72	D169	R247	
S73	E170	E248	
	R171	N249	
T78	F172	K250	
I79	K173		

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	108.12Å 108.12Å 160.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 50.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.00-2.90) 98.3 (50.00-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.75 (at 2.69Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.228 , 0.264 0.228 , 0.262	Depositor DCC
R_{free} test set	1021 reflections (3.80%)	wwPDB-VP
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5471	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.43	0/1913	0.98	7/2587 (0.3%)
1	B	0.45	0/1813	0.94	4/2454 (0.2%)
1	C	0.48	0/1837	0.99	6/2483 (0.2%)
All	All	0.45	0/5563	0.97	17/7524 (0.2%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	71	MSE	N-CA-C	9.04	124.30	112.72
1	C	13	TRP	N-CA-C	7.91	119.90	111.28
1	A	63	GLY	N-CA-C	-7.21	103.26	115.80
1	B	188	THR	N-CA-C	7.12	119.65	111.11
1	A	100	LEU	N-CA-C	-6.70	103.91	111.14
1	A	13	TRP	N-CA-C	6.68	118.64	111.36
1	A	17	TYR	N-CA-C	-6.67	103.26	111.33
1	B	231	PHE	N-CA-C	-6.62	105.17	113.18
1	A	211	ARG	CA-C-N	6.45	126.03	119.19
1	A	211	ARG	C-N-CA	6.45	126.03	119.19
1	A	117	ARG	N-CA-C	5.97	118.91	108.52
1	C	176	LEU	N-CA-C	-5.31	105.49	111.28
1	C	188	THR	N-CA-C	5.22	119.98	111.37
1	C	29	ILE	N-CA-C	5.19	116.05	108.53
1	B	133	LEU	N-CA-C	5.11	116.52	108.55
1	C	5	THR	N-CA-C	5.06	116.81	110.24
1	B	50	VAL	N-CA-C	5.02	118.58	112.80

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	1876	0	1836	137	0
1	B	1778	0	1742	95	0
1	C	1801	0	1763	80	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	10	0	0	0	0
All	All	5471	0	5341	307	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 28.

All (307) 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:188:THR:HG22	1:B:192:MSE:HE2	1.24	1.18
1:A:71:MSE:HE3	1:A:164:ARG:HH21	1.29	0.94
1:C:117:ARG:HH21	1:C:123:ASN:HD22	1.13	0.94
1:C:17:TYR:HB3	1:C:56:MSE:HE2	1.54	0.90
1:A:102:LEU:HB3	1:A:208:ILE:HD13	1.56	0.88
1:C:5:THR:HG23	1:C:8:GLU:HG3	1.55	0.88
1:A:247:ARG:HB3	1:A:247:ARG:HH11	1.40	0.85
1:A:102:LEU:HD13	1:A:208:ILE:HD11	1.58	0.84
1:B:106:LEU:HG	1:B:209:SER:HA	1.61	0.82
1:C:92:ILE:HD12	1:C:243:LEU:HD13	1.63	0.79
1:B:202:MSE:HE3	1:B:203:GLY:HA2	1.64	0.79
1:A:31:LEU:HD13	1:A:79:ILE:HD12	1.64	0.79
1:A:192:MSE:HG2	1:A:202:MSE:HE2	1.64	0.79
1:A:164:ARG:HA	1:A:213:MSE:HE2	1.66	0.78
1:A:98:GLY:HA2	1:A:212:PRO:HG3	1.66	0.77
1:B:115:ALA:HB2	1:B:192:MSE:HE1	1.67	0.77
1:A:20:ARG:HH21	1:A:60:SER:H	1.31	0.76
1:B:101:LYS:HE3	1:B:101:LYS:HA	1.67	0.76
1:C:117:ARG:HH21	1:C:123:ASN:ND2	1.85	0.75
1:A:19:GLN:HB3	1:A:50:VAL:HG12	1.69	0.74
1:C:149:LYS:NZ	1:C:237:MSE:HG2	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:ARG:NH2	1:C:123:ASN:HD22	1.85	0.73
1:A:18:THR:HB	1:A:58:ASN:ND2	2.03	0.73
1:A:12:ASN:O	1:A:15:PRO:HD2	1.89	0.73
1:B:17:TYR:HB3	1:B:56:MSE:HE2	1.71	0.72
1:B:5:THR:HG23	1:B:8:GLU:OE1	1.88	0.72
1:B:112:PRO:HB3	1:B:158:VAL:HG23	1.70	0.72
1:C:5:THR:HG23	1:C:8:GLU:CG	2.20	0.71
1:C:192:MSE:HG2	1:C:202:MSE:CE	2.21	0.71
1:C:192:MSE:HG2	1:C:202:MSE:HE1	1.72	0.70
1:A:20:ARG:NH2	1:A:60:SER:H	1.88	0.70
1:A:173:LYS:O	1:A:177:ARG:HG2	1.93	0.69
1:C:142:ILE:O	1:C:146:ILE:HG13	1.93	0.69
1:A:44:HIS:HD1	1:A:45:TYR:HD1	1.38	0.68
1:A:140:ARG:O	1:A:143:SER:HB3	1.93	0.68
1:A:32:THR:HG22	1:A:66:LEU:HD21	1.77	0.66
1:B:176:LEU:O	1:B:179:THR:HB	1.95	0.66
1:C:163:ARG:O	1:C:213:MSE:HE2	1.96	0.65
1:A:84:TRP:HB2	1:A:198:ASN:ND2	2.11	0.65
1:A:232:ALA:O	1:A:236:LEU:HB2	1.97	0.65
1:A:94:LEU:HD22	1:A:235:HIS:CD2	2.32	0.64
1:A:192:MSE:HG2	1:A:202:MSE:CE	2.27	0.64
1:A:126:LEU:HD12	1:A:193:THR:HG23	1.78	0.64
1:A:119:GLU:HG2	1:A:190:THR:OG1	1.98	0.64
1:B:115:ALA:CB	1:B:192:MSE:HE1	2.28	0.63
1:B:189:ALA:HA	1:B:192:MSE:HE3	1.81	0.63
1:B:202:MSE:HE3	1:B:203:GLY:CA	2.29	0.62
1:B:33:ASN:HB3	1:B:70:GLY:O	1.99	0.62
1:C:149:LYS:HZ2	1:C:237:MSE:HG2	1.63	0.62
1:A:109:TYR:HB3	1:A:205:LEU:HD11	1.81	0.62
1:A:202:MSE:HE3	1:A:203:GLY:HA2	1.81	0.62
1:C:73:SER:HB2	1:C:190:THR:OG1	1.99	0.62
1:C:188:THR:O	1:C:192:MSE:HG3	1.99	0.62
1:B:143:SER:O	1:B:147:GLN:HG3	1.99	0.62
1:B:116:ILE:HG12	1:B:179:THR:HG23	1.82	0.61
1:C:149:LYS:HZ1	1:C:241:ASP:CG	2.09	0.61
1:A:71:MSE:HE3	1:A:164:ARG:NH2	2.10	0.61
1:C:88:PRO:HG2	1:C:200:ILE:HG23	1.81	0.61
1:C:172:PHE:O	1:C:176:LEU:HD13	2.01	0.61
1:B:34:PHE:CE1	1:B:96:LYS:HG3	2.36	0.61
1:C:5:THR:HG23	1:C:8:GLU:CD	2.26	0.60
1:A:19:GLN:HB3	1:A:50:VAL:CG1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ARG:HD2	1:A:122:SER:OG	2.02	0.60
1:B:19:GLN:HG3	1:B:54:THR:HG21	1.84	0.59
1:C:32:THR:HG22	1:C:66:LEU:HD11	1.83	0.59
1:B:14:LEU:HB3	1:B:15:PRO:HD3	1.84	0.59
1:B:47:VAL:CG1	1:B:48:PRO:HD2	2.33	0.59
1:A:231:PHE:CD1	1:A:231:PHE:N	2.71	0.59
1:C:96:LYS:HE3	1:C:212:PRO:HA	1.85	0.59
1:C:100:LEU:HB2	1:C:182:SER:O	2.03	0.58
1:B:19:GLN:HG3	1:B:54:THR:CG2	2.32	0.58
1:B:52:GLU:HG2	1:B:53:HIS:ND1	2.18	0.58
1:A:32:THR:O	1:A:68:ASN:HA	2.04	0.58
1:B:192:MSE:HG2	1:B:202:MSE:CE	2.34	0.58
1:C:79:ILE:HD13	1:C:79:ILE:O	2.04	0.57
1:A:60:SER:HA	1:A:65:THR:HA	1.86	0.57
1:C:71:MSE:SE	1:C:215:PRO:HA	2.54	0.57
1:B:6:LYS:O	1:B:10:VAL:HG22	2.04	0.57
1:A:221:GLU:OE2	1:B:16:ARG:NH1	2.37	0.57
1:A:66:LEU:HD23	1:A:67:ILE:N	2.19	0.57
1:C:32:THR:CG2	1:C:66:LEU:HD11	2.35	0.57
1:A:5:THR:OG1	1:A:8:GLU:HG3	2.03	0.56
1:A:117:ARG:NH2	1:A:127:PRO:O	2.38	0.56
1:B:175:TYR:O	1:B:178:SER:N	2.39	0.56
1:A:202:MSE:HE3	1:A:203:GLY:CA	2.36	0.56
1:A:47:VAL:CG2	1:A:48:PRO:HD2	2.36	0.56
1:A:164:ARG:HA	1:A:213:MSE:CE	2.34	0.56
1:A:146:ILE:HG21	1:A:153:TYR:HD2	1.70	0.56
1:C:172:PHE:CZ	1:C:176:LEU:HD11	2.40	0.56
1:C:116:ILE:HD13	1:C:179:THR:HB	1.86	0.55
1:B:134:PRO:HA	1:B:202:MSE:HE2	1.88	0.55
1:A:247:ARG:HH11	1:A:247:ARG:CB	2.15	0.55
1:A:248:GLU:C	1:A:250:LYS:H	2.14	0.55
1:A:163:ARG:O	1:A:213:MSE:HE2	2.06	0.55
1:A:27:PRO:HG2	1:A:28:TYR:HD1	1.72	0.55
1:A:45:TYR:HD2	1:A:61:ALA:CB	2.20	0.54
1:A:88:PRO:HG2	1:A:200:ILE:HG23	1.88	0.54
1:B:179:THR:CG2	1:B:181:ALA:HB2	2.37	0.54
1:B:192:MSE:HG2	1:B:202:MSE:HE2	1.89	0.54
1:A:82:LEU:C	1:A:84:TRP:H	2.15	0.54
1:A:112:PRO:HD2	1:A:204:ALA:O	2.07	0.54
1:B:112:PRO:HB3	1:B:158:VAL:CG2	2.38	0.54
1:B:179:THR:HG22	1:B:181:ALA:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ILE:CD1	1:A:181:ALA:HB2	2.38	0.54
1:B:81:ASP:O	1:B:84:TRP:HB3	2.08	0.53
1:A:6:LYS:HG3	1:B:168:TYR:CE2	2.44	0.53
1:A:17:TYR:HB3	1:A:56:MSE:SE	2.59	0.53
1:C:146:ILE:HG21	1:C:153:TYR:CD2	2.43	0.53
1:A:94:LEU:HD22	1:A:235:HIS:NE2	2.24	0.53
1:B:11:GLU:HG2	1:B:22:LEU:HD21	1.91	0.53
1:B:47:VAL:HG13	1:B:48:PRO:HD2	1.89	0.53
1:A:47:VAL:HG23	1:A:48:PRO:HD2	1.89	0.53
1:B:10:VAL:HB	1:B:85:ALA:HB2	1.89	0.53
1:A:159:TYR:CD2	1:A:176:LEU:HD11	2.43	0.52
1:B:105:ALA:O	1:B:108:ASP:HB2	2.08	0.52
1:A:5:THR:HG23	1:A:8:GLU:OE1	2.10	0.52
1:B:147:GLN:C	1:B:149:LYS:H	2.17	0.52
1:B:166:TRP:C	1:B:168:TYR:H	2.17	0.52
1:C:15:PRO:O	1:C:19:GLN:N	2.41	0.52
1:A:14:LEU:HB3	1:A:15:PRO:HD3	1.92	0.52
1:A:66:LEU:HD23	1:A:66:LEU:C	2.35	0.52
1:A:188:THR:CG2	1:A:192:MSE:HE3	2.40	0.52
1:C:175:TYR:O	1:C:179:THR:HG23	2.10	0.52
1:C:80:MSE:HE3	1:C:195:GLY:HA3	1.92	0.52
1:A:100:LEU:CD2	1:A:176:LEU:HB3	2.39	0.51
1:A:116:ILE:HD12	1:A:181:ALA:HB2	1.91	0.51
1:C:92:ILE:HD12	1:C:243:LEU:CD1	2.38	0.51
1:C:179:THR:O	1:C:180:HIS:HB2	2.09	0.51
1:A:69:PHE:CG	1:A:79:ILE:HD13	2.45	0.51
1:A:25:PHE:CG	1:A:86:ILE:HD11	2.44	0.51
1:C:117:ARG:NH2	1:C:123:ASN:ND2	2.52	0.51
1:A:11:GLU:HG2	1:A:22:LEU:HD21	1.91	0.51
1:B:115:ALA:HB2	1:B:192:MSE:CE	2.39	0.51
1:B:15:PRO:HA	1:B:20:ARG:O	2.10	0.51
1:A:100:LEU:HD21	1:A:176:LEU:CG	2.40	0.51
1:A:71:MSE:HE2	1:A:215:PRO:CA	2.41	0.51
1:B:47:VAL:HG11	1:B:60:SER:O	2.11	0.51
1:B:115:ALA:CB	1:B:192:MSE:CE	2.89	0.50
1:B:140:ARG:O	1:B:143:SER:HB3	2.11	0.50
1:C:7:GLN:O	1:C:11:GLU:HB2	2.09	0.50
1:A:100:LEU:HD21	1:A:176:LEU:HD23	1.92	0.50
1:C:10:VAL:HB	1:C:85:ALA:HB2	1.94	0.50
1:A:20:ARG:HG2	1:A:20:ARG:HH11	1.75	0.50
1:A:241:ASP:O	1:A:245:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:TYR:O	1:B:176:LEU:C	2.54	0.50
1:C:80:MSE:CE	1:C:202:MSE:HG2	2.42	0.50
1:B:15:PRO:HG3	1:B:22:LEU:HD13	1.93	0.50
1:B:25:PHE:HE2	1:B:67:ILE:HD11	1.77	0.50
1:A:75:ASN:O	1:A:79:ILE:HG12	2.12	0.49
1:C:215:PRO:O	1:C:216:GLU:HG2	2.12	0.49
1:B:103:GLU:O	1:B:104:ASN:C	2.56	0.49
1:C:80:MSE:HE1	1:C:202:MSE:HG2	1.94	0.49
1:B:11:GLU:HG2	1:B:22:LEU:CD2	2.42	0.49
1:A:188:THR:O	1:A:192:MSE:HG3	2.13	0.49
1:A:46:GLY:O	1:A:47:VAL:HB	2.13	0.49
1:B:51:GLY:HA3	1:B:57:PRO:HA	1.95	0.49
1:C:177:ARG:HH11	1:C:177:ARG:HG2	1.77	0.49
1:B:179:THR:O	1:B:180:HIS:HB2	2.13	0.48
1:B:114:ALA:HB3	1:C:133:LEU:HD11	1.95	0.48
1:C:170:GLU:OE2	1:C:173:LYS:HE3	2.12	0.48
1:A:20:ARG:HH21	1:A:60:SER:N	2.07	0.48
1:B:100:LEU:HD11	1:B:184:VAL:HG23	1.95	0.48
1:C:211:ARG:N	1:C:212:PRO:CD	2.77	0.48
1:B:102:LEU:HB3	1:B:103:GLU:OE2	2.13	0.48
1:A:7:GLN:HG2	1:A:11:GLU:OE2	2.13	0.48
1:A:84:TRP:HB2	1:A:198:ASN:HD22	1.77	0.48
1:C:19:GLN:HB2	1:C:54:THR:HG21	1.95	0.48
1:C:10:VAL:HG23	1:C:11:GLU:N	2.29	0.48
1:C:15:PRO:HA	1:C:20:ARG:O	2.14	0.48
1:A:40:VAL:HG11	1:A:233:GLU:HG2	1.95	0.48
1:B:29:ILE:HG22	1:B:30:LEU:N	2.28	0.47
1:B:14:LEU:CD2	1:B:86:ILE:HD12	2.43	0.47
1:B:231:PHE:O	1:B:233:GLU:N	2.48	0.47
1:A:39:HIS:O	1:A:40:VAL:C	2.58	0.47
1:C:34:PHE:HZ	1:C:96:LYS:HB3	1.79	0.47
1:A:5:THR:O	1:A:9:ILE:HG13	2.15	0.47
1:A:10:VAL:HG11	1:A:81:ASP:O	2.15	0.47
1:A:125:TYR:O	1:A:126:LEU:HD23	2.15	0.47
1:A:44:HIS:CD2	1:A:237:MSE:HE1	2.50	0.47
1:A:20:ARG:HG2	1:A:20:ARG:NH1	2.29	0.47
1:A:233:GLU:O	1:A:237:MSE:HG2	2.13	0.47
1:C:140:ARG:HG2	1:C:140:ARG:HH11	1.79	0.47
1:C:20:ARG:HD2	1:C:25:PHE:CE2	2.50	0.46
1:B:14:LEU:HD21	1:B:86:ILE:HD12	1.98	0.46
1:C:174:ASP:O	1:C:177:ARG:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:PHE:O	1:B:232:ALA:C	2.57	0.46
1:C:192:MSE:HE2	1:C:202:MSE:HE1	1.96	0.46
1:B:18:THR:O	1:B:19:GLN:HB2	2.14	0.46
1:B:109:TYR:CE2	1:B:207:LEU:HD13	2.50	0.46
1:B:116:ILE:HD12	1:B:116:ILE:N	2.30	0.46
1:A:27:PRO:HG2	1:A:28:TYR:CD1	2.51	0.46
1:A:222:GLU:OE1	1:A:222:GLU:HA	2.14	0.46
1:B:29:ILE:HB	1:B:91:VAL:HG22	1.97	0.46
1:C:34:PHE:HD1	1:C:37:TYR:CE1	2.34	0.46
1:C:231:PHE:CD1	1:C:231:PHE:N	2.84	0.46
1:A:29:ILE:HG22	1:A:30:LEU:N	2.30	0.45
1:B:32:THR:O	1:B:68:ASN:HA	2.16	0.45
1:B:104:ASN:O	1:B:105:ALA:HB3	2.16	0.45
1:C:233:GLU:O	1:C:237:MSE:HB2	2.17	0.45
1:A:140:ARG:HG2	1:A:140:ARG:HH11	1.79	0.45
1:A:115:ALA:HB1	1:A:189:ALA:HB2	1.98	0.45
1:B:140:ARG:HH12	1:C:147:GLN:CD	2.25	0.45
1:A:28:TYR:HB3	1:A:243:LEU:HD13	1.99	0.45
1:A:31:LEU:CD2	1:A:67:ILE:HB	2.47	0.45
1:A:41:PHE:HE1	1:A:240:ILE:HD11	1.81	0.45
1:A:248:GLU:C	1:A:250:LYS:N	2.75	0.45
1:B:50:VAL:HG22	1:B:58:ASN:OD1	2.17	0.45
1:A:94:LEU:HB3	1:A:235:HIS:NE2	2.32	0.45
1:C:172:PHE:CE2	1:C:176:LEU:HD11	2.51	0.45
1:A:44:HIS:ND1	1:A:45:TYR:CE1	2.84	0.45
1:A:119:GLU:O	1:A:121:THR:N	2.46	0.45
1:A:168:TYR:CD1	1:A:168:TYR:C	2.94	0.45
1:B:31:LEU:HD23	1:B:67:ILE:HB	1.98	0.45
1:A:5:THR:HG23	1:A:8:GLU:CD	2.42	0.44
1:A:70:GLY:O	1:A:71:MSE:C	2.60	0.44
1:C:47:VAL:HG11	1:C:61:ALA:HB2	1.99	0.44
1:B:25:PHE:HB2	1:B:86:ILE:HD13	1.99	0.44
1:C:100:LEU:HD11	1:C:184:VAL:HG23	1.99	0.44
1:A:100:LEU:HD21	1:A:176:LEU:HB3	1.99	0.44
1:B:167:GLU:OE1	1:B:167:GLU:N	2.45	0.44
1:A:18:THR:HB	1:A:58:ASN:HD21	1.79	0.44
1:A:164:ARG:HG2	1:A:213:MSE:HE3	1.99	0.44
1:B:104:ASN:CG	1:B:105:ALA:H	2.25	0.44
1:A:102:LEU:HD13	1:A:208:ILE:CD1	2.38	0.44
1:B:60:SER:O	1:B:61:ALA:HB2	2.18	0.43
1:A:56:MSE:HA	1:A:68:ASN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:PHE:CZ	1:B:96:LYS:HG3	2.53	0.43
1:C:78:THR:O	1:C:82:LEU:HG	2.19	0.43
1:C:248:GLU:O	1:C:250:LYS:N	2.52	0.43
1:A:20:ARG:HH21	1:A:59:ALA:HA	1.84	0.43
1:A:151:LYS:HE3	1:A:234:GLU:OE2	2.19	0.43
1:B:208:ILE:HG22	1:B:209:SER:N	2.33	0.43
1:A:60:SER:HB3	1:A:65:THR:HG23	2.00	0.43
1:B:135:SER:HB3	1:B:138:VAL:CG2	2.49	0.43
1:C:18:THR:HG22	1:C:56:MSE:HE3	1.99	0.43
1:A:71:MSE:HE1	1:A:213:MSE:O	2.18	0.43
1:C:11:GLU:HG2	1:C:22:LEU:HD11	1.99	0.43
1:A:71:MSE:HG3	1:A:215:PRO:HA	2.00	0.43
1:B:45:TYR:O	1:B:47:VAL:HG23	2.19	0.43
1:B:136:PHE:HB3	1:C:155:THR:HG21	2.00	0.43
1:A:14:LEU:HD13	1:A:82:LEU:HB3	2.01	0.43
1:A:26:GLU:OE1	1:A:63:GLY:HA2	2.19	0.43
1:A:44:HIS:CE1	1:A:45:TYR:HE1	2.37	0.43
1:A:98:GLY:HA2	1:A:212:PRO:CG	2.43	0.43
1:B:165:VAL:HG12	1:B:168:TYR:HE2	1.84	0.43
1:B:18:THR:C	1:B:20:ARG:H	2.26	0.42
1:C:248:GLU:O	1:C:249:ASN:C	2.61	0.42
1:A:39:HIS:C	1:A:41:PHE:N	2.76	0.42
1:A:82:LEU:C	1:A:84:TRP:N	2.75	0.42
1:A:231:PHE:H	1:A:231:PHE:HD1	1.67	0.42
1:A:38:LEU:HG	1:A:49:ILE:HD12	2.02	0.42
1:A:110:LEU:O	1:A:112:PRO:HD3	2.19	0.42
1:C:71:MSE:HE2	1:C:186:MSE:CE	2.50	0.42
1:A:71:MSE:HE2	1:A:215:PRO:HA	2.01	0.42
1:C:35:SER:HA	1:C:68:ASN:HD22	1.84	0.42
1:B:51:GLY:O	1:B:53:HIS:N	2.51	0.42
1:B:10:VAL:CB	1:B:85:ALA:HB2	2.50	0.42
1:C:144:SER:O	1:C:145:ALA:C	2.62	0.42
1:C:147:GLN:O	1:C:150:GLY:N	2.38	0.42
1:C:168:TYR:CD1	1:C:168:TYR:C	2.98	0.42
1:A:45:TYR:HD2	1:A:61:ALA:HB3	1.84	0.42
1:A:109:TYR:N	1:A:109:TYR:CD1	2.88	0.42
1:C:215:PRO:O	1:C:216:GLU:CG	2.68	0.42
1:A:41:PHE:HE2	1:A:59:ALA:O	2.02	0.41
1:B:50:VAL:O	1:B:50:VAL:HG23	2.20	0.41
1:A:19:GLN:CB	1:A:50:VAL:HG12	2.45	0.41
1:A:186:MSE:SE	1:A:213:MSE:HE3	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:PHE:CE2	1:B:67:ILE:HD11	2.55	0.41
1:A:21:GLN:HB2	1:A:24:ASP:OD2	2.20	0.41
1:A:136:PHE:O	1:A:137:SER:C	2.63	0.41
1:A:142:ILE:O	1:A:146:ILE:HG13	2.21	0.41
1:A:241:ASP:O	1:A:244:GLU:HB3	2.20	0.41
1:C:12:ASN:HD21	1:C:16:ARG:NH1	2.18	0.41
1:B:91:VAL:O	1:B:202:MSE:HA	2.20	0.41
1:B:116:ILE:HG12	1:B:179:THR:CG2	2.50	0.41
1:C:26:GLU:OE1	1:C:63:GLY:HA2	2.20	0.41
1:C:34:PHE:CZ	1:C:96:LYS:HD3	2.55	0.41
1:A:43:GLU:C	1:A:45:TYR:N	2.77	0.41
1:A:166:TRP:C	1:A:168:TYR:H	2.27	0.41
1:B:13:TRP:O	1:B:14:LEU:C	2.61	0.41
1:A:69:PHE:HB3	1:A:79:ILE:HG21	2.02	0.41
1:A:76:ALA:HB2	1:A:187:GLU:HB2	2.03	0.41
1:A:100:LEU:HD21	1:A:176:LEU:CD2	2.51	0.41
1:C:91:VAL:O	1:C:202:MSE:HA	2.20	0.41
1:A:26:GLU:HB3	1:A:63:GLY:O	2.19	0.41
1:B:151:LYS:HG3	1:B:152:ASP:H	1.85	0.41
1:B:231:PHE:C	1:B:233:GLU:N	2.78	0.41
1:A:71:MSE:HE2	1:A:214:PHE:C	2.46	0.41
1:A:110:LEU:HD21	1:A:158:VAL:HG13	2.01	0.41
1:B:13:TRP:HB2	1:B:82:LEU:HD22	2.03	0.41
1:B:104:ASN:OD1	1:B:105:ALA:N	2.39	0.41
1:B:233:GLU:O	1:B:234:GLU:C	2.63	0.41
1:C:79:ILE:O	1:C:83:LEU:HG	2.21	0.41
1:C:215:PRO:O	1:C:216:GLU:CB	2.69	0.41
1:A:111:LEU:HD12	1:A:111:LEU:HA	1.94	0.41
1:B:166:TRP:C	1:B:168:TYR:N	2.79	0.41
1:C:105:ALA:HB1	1:C:108:ASP:OD2	2.20	0.41
1:C:169:ASP:OD1	1:C:169:ASP:C	2.63	0.41
1:A:40:VAL:CG1	1:A:233:GLU:HG2	2.52	0.40
1:B:12:ASN:O	1:B:16:ARG:HD3	2.22	0.40
1:B:68:ASN:OD1	1:B:68:ASN:C	2.64	0.40
1:C:192:MSE:HG2	1:C:202:MSE:HE2	2.02	0.40
1:B:188:THR:HG22	1:B:192:MSE:CE	2.18	0.40
1:A:12:ASN:C	1:A:15:PRO:HD2	2.45	0.40
1:A:115:ALA:O	1:A:132:SER:HB2	2.21	0.40
1:B:164:ARG:HG2	1:B:186:MSE:SE	2.72	0.40
1:C:20:ARG:HD2	1:C:25:PHE:CZ	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	236/268 (88%)	200 (85%)	27 (11%)	9 (4%)	2	10
1	B	224/268 (84%)	196 (88%)	21 (9%)	7 (3%)	3	14
1	C	224/268 (84%)	202 (90%)	17 (8%)	5 (2%)	5	20
All	All	684/804 (85%)	598 (87%)	65 (10%)	21 (3%)	3	14

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	52	GLU
1	C	215	PRO
1	A	120	GLY
1	B	104	ASN
1	A	71	MSE
1	A	249	ASN
1	B	232	ALA
1	C	167	GLU
1	C	249	ASN
1	A	222	GLU
1	B	102	LEU
1	B	148	ASN
1	B	167	GLU
1	C	148	ASN
1	C	248	GLU
1	A	62	GLU
1	A	83	LEU
1	B	169	ASP
1	A	134	PRO
1	A	9	ILE
1	A	215	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	200/222 (90%)	188 (94%)	12 (6%)	17	47
1	B	189/222 (85%)	179 (95%)	10 (5%)	20	52
1	C	191/222 (86%)	177 (93%)	14 (7%)	13	38
All	All	580/666 (87%)	544 (94%)	36 (6%)	16	46

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	79	ILE
1	A	119	GLU
1	A	129	GLU
1	A	158	VAL
1	A	176	LEU
1	A	187	GLU
1	A	202	MSE
1	A	220	THR
1	A	231	PHE
1	A	236	LEU
1	A	247	ARG
1	B	5	THR
1	B	33	ASN
1	B	50	VAL
1	B	101	LYS
1	B	119	GLU
1	B	121	THR
1	B	155	THR
1	B	176	LEU
1	B	185	ASP
1	B	202	MSE
1	C	5	THR
1	C	38	LEU
1	C	40	VAL
1	C	50	VAL

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Mol	Chain	Res	Type
1	C	79	ILE
1	C	106	LEU
1	C	117	ARG
1	C	119	GLU
1	C	128	GLU
1	C	155	THR
1	C	202	MSE
1	C	231	PHE
1	C	243	LEU
1	C	247	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	123	ASN
1	A	148	ASN
1	A	162	ASN
1	A	198	ASN
1	A	249	ASN
1	B	7	GLN
1	B	36	HIS
1	B	148	ASN
1	C	19	GLN
1	C	39	HIS
1	C	53	HIS
1	C	75	ASN
1	C	123	ASN
1	C	148	ASN
1	C	162	ASN

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 [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 [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	232/268 (86%)	0.67	15 (6%) 25 20	28, 55, 70, 78	0
1	B	221/268 (82%)	0.00	2 (0%) 81 75	20, 37, 57, 75	0
1	C	222/268 (82%)	-0.08	1 (0%) 87 83	15, 33, 51, 67	0
All	All	675/804 (83%)	0.21	18 (2%) 56 47	15, 40, 67, 78	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	230	ASN	3.6
1	A	98	GLY	3.3
1	A	102	LEU	2.8
1	B	209	SER	2.7
1	B	102	LEU	2.7
1	A	230	ASN	2.6
1	A	5	THR	2.5
1	A	79	ILE	2.4
1	A	61	ALA	2.3
1	A	48	PRO	2.2
1	A	13	TRP	2.2
1	A	35	SER	2.2
1	A	86	ILE	2.1
1	A	250	LYS	2.1
1	A	249	ASN	2.1
1	A	28	TYR	2.1
1	A	70	GLY	2.0
1	A	99	GLY	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.