



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:41 PM GMT

PDB ID : 1YBF
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

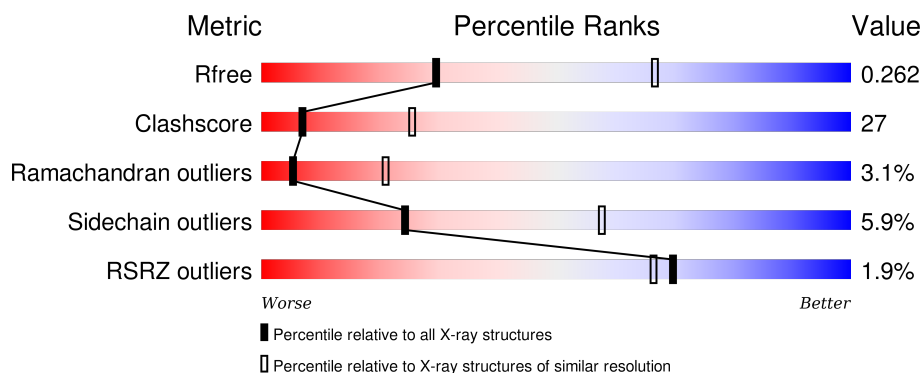
1 Overall quality at a glance

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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>4%</div> <div>41% 44% 10%</div> </div>
1	B	268	<div> <div>%</div> <div>48% 32% 15%</div> </div>
1	C	268	<div> <div></div> <div>51% 31% 14%</div> </div>

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			

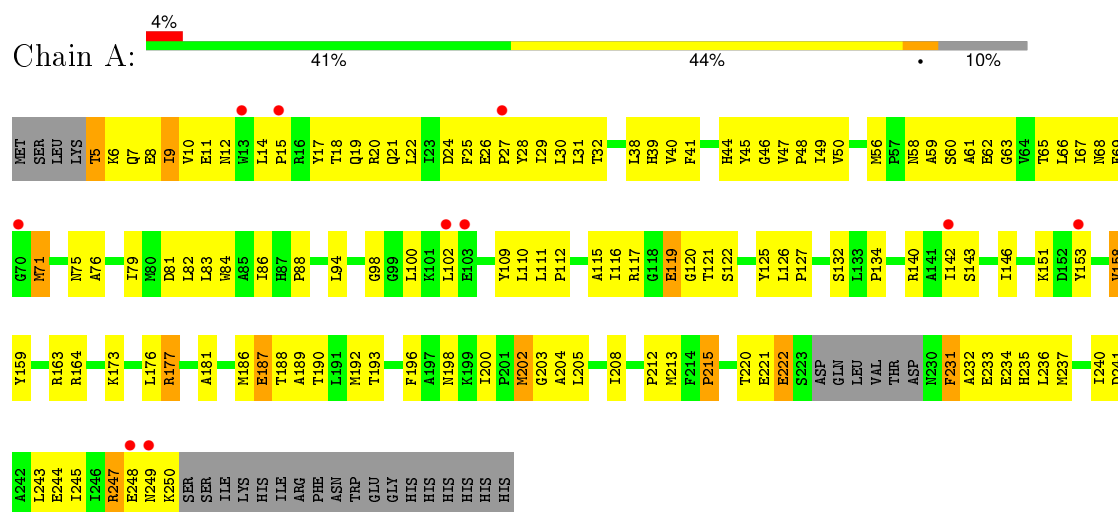
- Molecule 2 is water.

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		

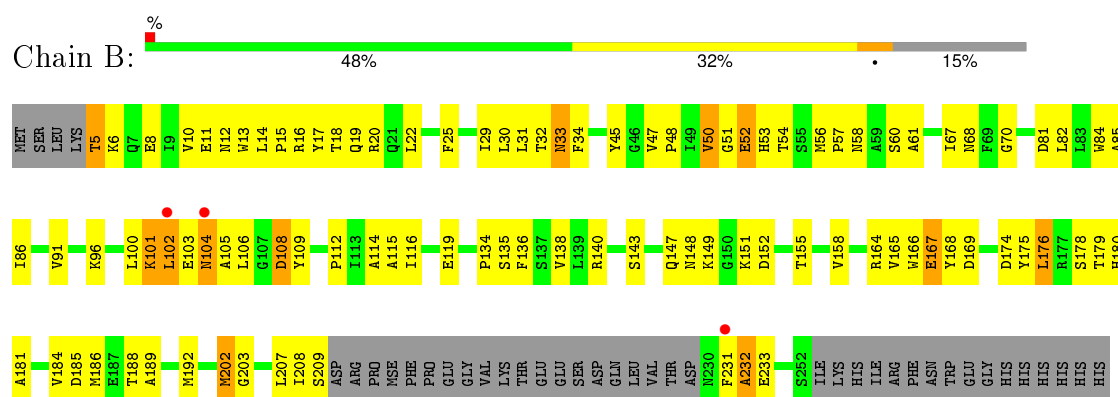
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

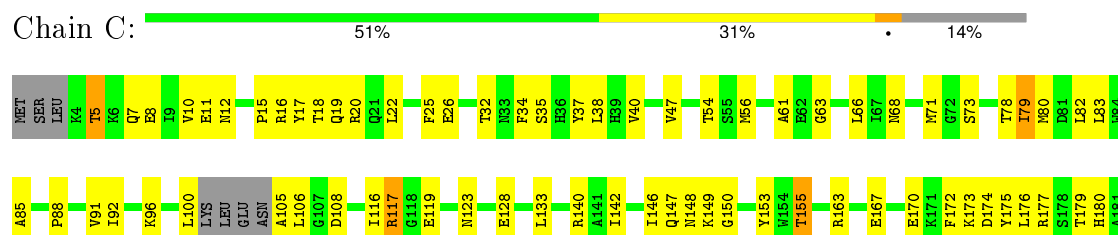
• Molecule 1: AMP nucleosidase



• Molecule 1: AMP nucleosidase



• Molecule 1: AMP nucleosidase



S182	G183	V184	D185	M186	E187	T188	A189	T190	L191	M192	G195	T200	P201	M202	R211	P212	M213	F214	P215	E216	GLY	VAL	LYS	THR	GLU	GLU	SER	ASP	GLN	LEU	VAL	THR	ASP	N230	F231	A232	E233	M237	D241	A242	L243	R247	F248	N249	R250	SER	SER	ILE	LYS	HIS	ILE	ARG	PHE
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----

ASN	TRP	GLU	GLY	HIS	HIS	HIS	HIS	HIS
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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 46.30 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.00-2.90) 97.1 (46.30-2.70)	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 (4.76%)	DCC
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 26895 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.37	0/1913	0.62	0/2587
1	B	0.39	0/1813	0.63	0/2454
1	C	0.41	0/1837	0.64	0/2483
All	All	0.39	0/5563	0.63	0/7524

There are no bond length outliers.

There are no bond angle outliers.

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	128	0
1	B	1778	0	1742	87	0
1	C	1801	0	1763	76	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	287	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 27.

All (287) 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:C:5:THR:HG23	1:C:8:GLU:HG3	1.55	0.88
1:A:102:LEU:HB3	1:A:208:ILE:HD13	1.56	0.88
1:A:247:ARG:HH11	1:A:247:ARG:HB3	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:202:MSE:HE3	1:A:203:GLY:HA2	1.81	0.62
1:A:109:TYR:HB3	1:A:205:LEU:HD11	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: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:A:19:GLN:HB3	1:A:50:VAL:CG1	2.32	0.60
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:N	1:A:231:PHE:CD1	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:B:192:MSE:HG2	1:B:202:MSE:CE	2.34	0.58
1:A:32:THR:O	1:A:68:ASN:HA	2.04	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:B:175:TYR:O	1:B:178:SER:N	2.39	0.56
1:A:117:ARG:NH2	1:A:127:PRO:O	2.38	0.56
1:A:202:MSE:HE3	1:A:203:GLY:CA	2.36	0.56
1:A:164:ARG:HA	1:A:213:MSE:CE	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:VAL:CG2	1:A:48:PRO:HD2	2.36	0.56
1:C:5:THR:HG23	1:C:8:GLU:CD	2.26	0.56
1:C:172:PHE:CZ	1:C:176:LEU:HD11	2.40	0.56
1:A:146:ILE:HG21	1:A:153:TYR:HD2	1.70	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: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:C:149:LYS:HZ3	1:C:237:MSE:HG2	1.73	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
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:17:TYR:HB3	1:A:56:MSE:SE	2.59	0.53
1:A:6:LYS:HG3	1:B:168:TYR:CE2	2.44	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:B:10:VAL:HB	1:B:85:ALA:HB2	1.89	0.53
1:A:47:VAL:HG23	1:A:48:PRO:HD2	1.89	0.53
1:A:132:SER:HG	1:A:193:THR:HG1	1.57	0.52
1:B:105:ALA:O	1:B:108:ASP:HB2	2.08	0.52
1:A:159:TYR:CD2	1:A:176:LEU:HD11	2.43	0.52
1:A:5:THR:HG23	1:A:8:GLU:OE1	2.10	0.52
1:C:15:PRO:O	1:C:19:GLN:N	2.41	0.52
1:A:188:THR:CG2	1:A:192:MSE:HE3	2.40	0.52
1:A:14:LEU:HB3	1:A:15:PRO:HD3	1.92	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: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:116:ILE:HD12	1:A:181:ALA:HB2	1.91	0.51
1:A:100:LEU:CD2	1:A:176:LEU:HB3	2.39	0.51
1:A:69:PHE:CG	1:A:79:ILE:HD13	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:ARG:NH2	1:C:123:ASN:ND2	2.52	0.51
1:A:25:PHE:CG	1:A:86:ILE:HD11	2.44	0.51
1:B:115:ALA:HB2	1:B:192:MSE:CE	2.39	0.51
1:A:11:GLU:HG2	1:A:22:LEU:HD21	1.91	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:A:248:GLU:C	1:A:250:LYS:H	2.14	0.50
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:HH11	1:A:20:ARG:HG2	1.75	0.50
1:A:241:ASP:O	1:A:245:ILE:HG13	2.11	0.50
1:C:149:LYS:HZ2	1:C:237:MSE:HG2	1.75	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:A:82:LEU:C	1:A:84:TRP:H	2.15	0.49
1:C:215:PRO:O	1:C:216:GLU:HG2	2.12	0.49
1:C:80:MSE:HE1	1:C:202:MSE:HG2	1.94	0.49
1:B:179:THR:O	1:B:180:HIS:HB2	2.13	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:HG2	1:C:177:ARG:HH11	1.77	0.49
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:84:TRP:HB2	1:A:198:ASN:HD22	1.77	0.48
1:B:147:GLN:C	1:B:149:LYS:H	2.17	0.48
1:A:7:GLN:HG2	1:A:11:GLU:OE2	2.13	0.48
1:C:19:GLN:HB2	1:C:54:THR:HG21	1.95	0.48
1:C:15:PRO:HA	1:C:20:ARG:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:VAL:HG23	1:C:11:GLU:N	2.29	0.48
1:A:40:VAL:HG11	1:A:233:GLU:HG2	1.95	0.48
1:B:166:TRP:C	1:B:168:TYR:H	2.17	0.47
1:B:29:ILE:HG22	1:B:30:LEU:N	2.28	0.47
1:A:66:LEU:C	1:A:66:LEU:HD23	2.35	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:C:34:PHE:HZ	1:C:96:LYS:HB3	1.79	0.47
1:A:125:TYR:O	1:A:126:LEU:HD23	2.15	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: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
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:116:ILE:N	1:B:116:ILE:HD12	2.30	0.46
1:B:109:TYR:CE2	1:B:207:LEU:HD13	2.50	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:A:27:PRO:HG2	1:A:28:TYR:CD1	2.51	0.46
1:C:231:PHE:CD1	1:C:231:PHE:N	2.84	0.46
1:A:222:GLU:OE1	1:A:222:GLU:HA	2.14	0.46
1:C:233:GLU:O	1:C:237:MSE:HB2	2.17	0.45
1:B:175:TYR:O	1:B:176:LEU:C	2.54	0.45
1:B:104:ASN:O	1:B:105:ALA:HB3	2.16	0.45
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: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: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:28:TYR:HB3	1:A:243:LEU:HD13	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLU:O	1:A:121:THR:N	2.46	0.45
1:B:31:LEU:HD23	1:B:67:ILE:HB	1.98	0.45
1:B:103:GLU:O	1:B:104:ASN:C	2.56	0.45
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: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
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:B:208:ILE:HG22	1:B:209:SER:N	2.33	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:C:18:THR:HG22	1:C:56:MSE:HE3	1.99	0.43
1:A:60:SER:HB3	1:A:65:THR:HG23	2.00	0.43
1:C:149:LYS:HZ1	1:C:241:ASP:CG	2.22	0.43
1:B:135:SER:HB3	1:B:138:VAL:CG2	2.49	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:98:GLY:HA2	1:A:212:PRO:CG	2.43	0.43
1:A:14:LEU:HD13	1:A:82:LEU:HB3	2.01	0.43
1:A:44:HIS:CE1	1:A:45:TYR:HE1	2.37	0.43
1:B:165:VAL:HG12	1:B:168:TYR:HE2	1.84	0.43
1:A:26:GLU:OE1	1:A:63:GLY:HA2	2.19	0.43
1:A:39:HIS:O	1:A:40:VAL:C	2.58	0.42
1:A:231:PHE:HD1	1:A:231:PHE:H	1.67	0.42
1:C:71:MSE:HE2	1:C:186:MSE:CE	2.50	0.42
1:A:110:LEU:O	1:A:112:PRO:HD3	2.19	0.42
1:A:38:LEU:HG	1:A:49:ILE:HD12	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:VAL:CB	1:B:85:ALA:HB2	2.50	0.42
1:C:147:GLN:O	1:C:150:GLY:N	2.38	0.42
1:A:45:TYR:HD2	1:A:61:ALA:HB3	1.84	0.42
1:A:109:TYR:CD1	1:A:109:TYR:N	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:231:PHE:O	1:B:232:ALA:C	2.57	0.41
1:B:50:VAL:O	1:B:50:VAL:HG23	2.20	0.41
1:A:186:MSE:SE	1:A:213:MSE:HE3	2.69	0.41
1:A:19:GLN:CB	1:A:50:VAL:HG12	2.45	0.41
1:B:25:PHE:CE2	1:B:67:ILE:HD11	2.55	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:A:21:GLN:HB2	1:A:24:ASP:OD2	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:34:PHE:CZ	1:C:96:LYS:HD3	2.55	0.41
1:C:26:GLU:OE1	1:C:63:GLY:HA2	2.20	0.41
1:A:69:PHE:HB3	1:A:79:ILE:HG21	2.02	0.41
1:C:91:VAL:O	1:C:202:MSE:HA	2.20	0.41
1:A:100:LEU:HD21	1:A:176:LEU:CD2	2.51	0.41
1:A:76:ALA:HB2	1:A:187:GLU:HB2	2.03	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: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:110:LEU:HD21	1:A:158:VAL:HG13	2.01	0.41
1:B:104:ASN:OD1	1:B:105:ALA:N	2.39	0.41
1:B:13:TRP:HB2	1:B:82:LEU:HD22	2.03	0.41
1:A:111:LEU:HD12	1:A:111:LEU:HA	1.94	0.41
1:C:105:ALA:HB1	1:C:108:ASP:OD2	2.20	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:A:248:GLU:C	1:A:250:LYS:N	2.75	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:115:ALA:O	1:A:132:SER:HB2	2.21	0.40
1:C:20:ARG:HD2	1:C:25:PHE:CZ	2.56	0.40
1:B:164:ARG:HG2	1:B:186:MSE:SE	2.72	0.40

There are no symmetry-related clashes.

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	236/268 (88%)	200 (85%)	27 (11%)	9 (4%)	4	16
1	B	224/268 (84%)	196 (88%)	21 (9%)	7 (3%)	5	21
1	C	224/268 (84%)	202 (90%)	17 (8%)	5 (2%)	8	31
All	All	684/804 (85%)	598 (87%)	65 (10%)	21 (3%)	5	21

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%)	190 (95%)	10 (5%)	30	65
1	B	189/222 (85%)	178 (94%)	11 (6%)	25	58
1	C	191/222 (86%)	178 (93%)	13 (7%)	20	49
All	All	580/666 (87%)	546 (94%)	34 (6%)	24	58

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	119	GLU
1	A	158	VAL
1	A	177	ARG
1	A	187	GLU
1	A	196	PHE
1	A	202	MSE
1	A	220	THR
1	A	231	PHE
1	A	247	ARG
1	B	5	THR
1	B	33	ASN
1	B	50	VAL
1	B	101	LYS
1	B	108	ASP
1	B	119	GLU
1	B	155	THR
1	B	174	ASP
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	79	ILE
1	C	106	LEU

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Mol	Chain	Res	Type
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) 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	B	7	GLN
1	B	36	HIS
1	B	39	HIS
1	B	148	ASN
1	C	33	ASN
1	C	53	HIS
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 ⓘ

There are no carbohydrates 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 [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%)	0.38	10 (4%) 39 32	28, 55, 70, 78	0
1	B	221/268 (82%)	-0.14	3 (1%) 78 76	20, 37, 57, 75	0
1	C	222/268 (82%)	-0.25	0 100 100	15, 33, 51, 67	0
All	All	675/804 (83%)	0.00	13 (1%) 70 66	15, 40, 67, 78	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	102	LEU	4.5
1	A	102	LEU	3.8
1	B	104	ASN	3.2
1	A	15	PRO	2.9
1	A	142	ILE	2.7
1	A	13	TRP	2.6
1	A	249	ASN	2.5
1	A	103	GLU	2.5
1	A	248	GLU	2.2
1	A	27	PRO	2.1
1	A	153	TYR	2.1
1	B	231	PHE	2.0
1	A	70	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 carbohydrates 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.