



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:53 AM UTC

PDB ID : 1OKJ / pdb_00001okj
Title : crystal structure of the essential E. coli YeaZ protein by MAD method using the gadolinium complex "DOTMA"
Authors : Abergel, C.; Jeudy, S.; Claverie, J.M.
Deposited on : 2003-07-26
Resolution : 2.28 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

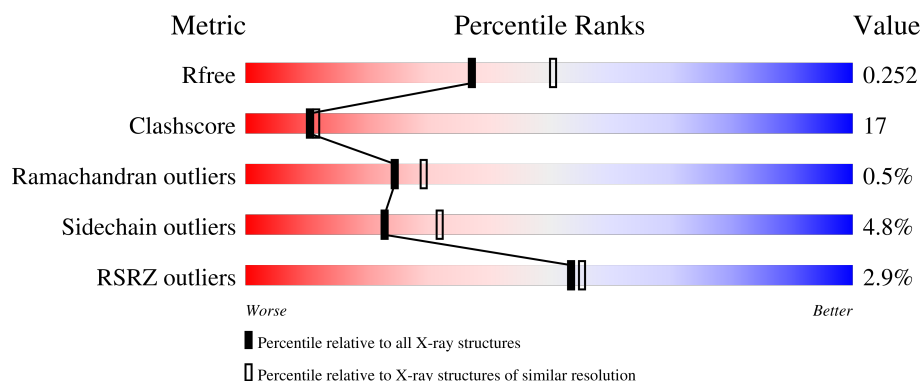
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	251	5% 58% 25% 5% 12%
1	B	251	% 70% 16% • 11%
1	C	251	2% 58% 27% • 13%
1	D	251	2% 57% 25% 5% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6983 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 TRNA THREONYLCARBAMOYLADENOSINE BIOSYNTHESIS PROTEIN TSAB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	1
			1663	1048	288	316	11			
1	B	223	Total	C	N	O	S	0	0	1
			1686	1063	293	319	11			
1	C	219	Total	C	N	O	S	0	0	1
			1655	1042	287	315	11			
1	D	221	Total	C	N	O	S	0	0	1
			1668	1051	289	317	11			

- Molecule 2 is GADOLINIUM ION (CCD ID: GD3) (formula: Gd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	8	Total	Gd	0	0
			8	8		

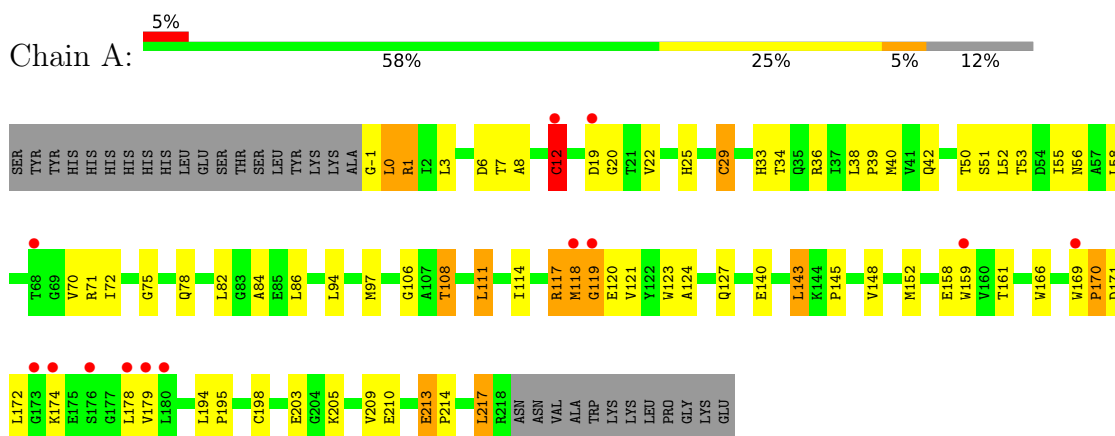
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	64	Total	O	0	0
			64	64		
3	B	95	Total	O	0	0
			95	95		
3	C	66	Total	O	0	0
			66	66		
3	D	78	Total	O	0	0
			78	78		

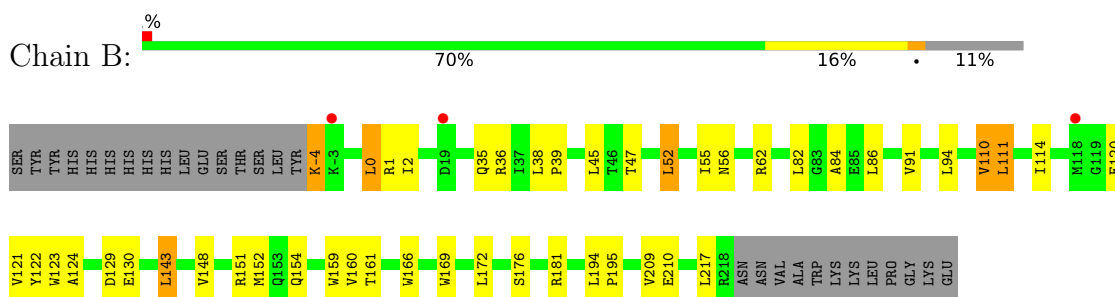
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

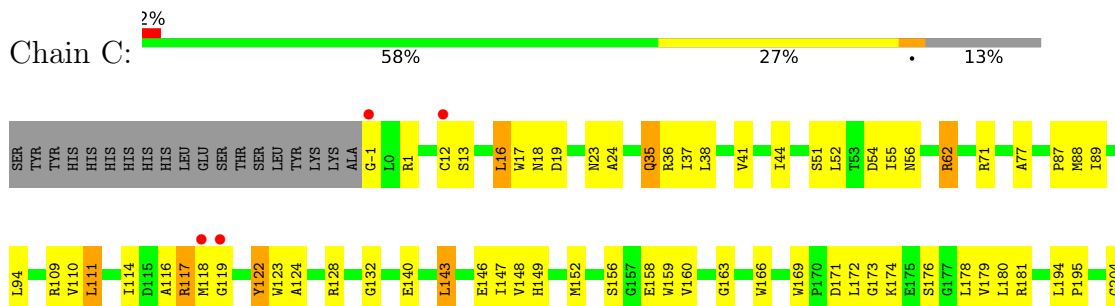
- Molecule 1: TRNA THREONYLCARBAMOYLADENOSINE BIOSYNTHESIS PROTEIN TSAB

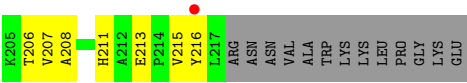


- Molecule 1: TRNA THREONYLCARBAMOYLADENOSINE BIOSYNTHESIS PROTEIN TSAB

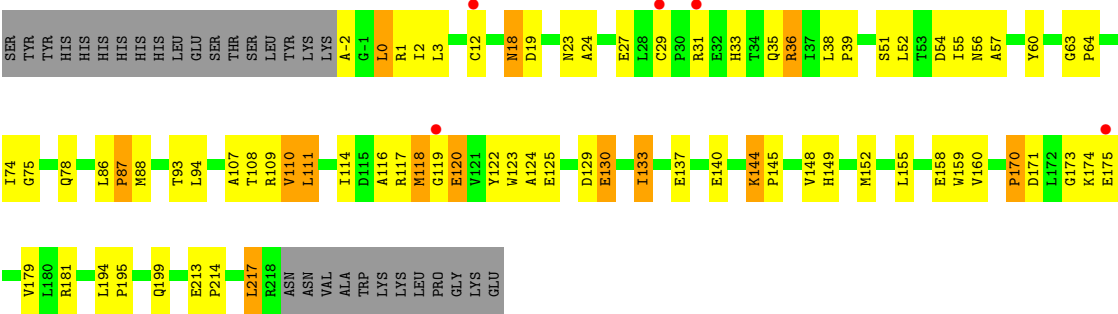


- Molecule 1: TRNA THREONYLCARBAMOYLADENOSINE BIOSYNTHESIS PROTEIN TSAB





● Molecule 1: TRNA THREONYLCARBAMOYLADENOSINE BIOSYNTHESIS PROTEIN TSAB



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.34Å 97.60Å 141.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.28 20.00 – 2.28	Depositor EDS
% Data completeness (in resolution range)	98.3 (20.00-2.28) 98.2 (20.00-2.28)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.13 (at 2.28Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.216 , 0.257 0.210 , 0.252	Depositor DCC
R_{free} test set	4871 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6983	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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: GD3

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	1/1697 (0.1%)	0.93	6/2311 (0.3%)
1	B	0.46	1/1720 (0.1%)	0.93	7/2340 (0.3%)
1	C	0.41	1/1689 (0.1%)	0.96	10/2300 (0.4%)
1	D	0.44	1/1702 (0.1%)	0.94	6/2318 (0.3%)
All	All	0.44	4/6808 (0.1%)	0.94	29/9269 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	217	LEU	C-N	-5.57	1.25	1.33
1	A	217	LEU	C-N	-5.54	1.25	1.33
1	B	217	LEU	C-N	-5.52	1.25	1.33
1	C	216	TYR	C-N	-5.51	1.25	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	119	GLY	N-CA-C	-10.24	100.51	114.95
1	A	213	GLU	N-CA-C	9.29	116.33	108.07
1	C	110	VAL	N-CA-C	7.08	118.03	108.11
1	D	110	VAL	N-CA-C	6.64	118.16	108.53
1	A	119	GLY	N-CA-C	-6.61	104.31	115.62
1	C	169	TRP	CA-C-N	6.31	125.81	119.24
1	C	169	TRP	C-N-CA	6.31	125.81	119.24
1	C	13	SER	N-CA-C	6.22	118.63	109.24
1	B	82	LEU	N-CA-C	6.11	117.62	110.97
1	D	120	GLU	N-CA-C	6.03	117.74	109.18
1	B	110	VAL	N-CA-C	5.97	116.47	108.11
1	B	169	TRP	CA-C-N	5.75	125.87	119.32
1	B	169	TRP	C-N-CA	5.75	125.87	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	PRO	N-CA-C	-5.66	107.41	114.20
1	B	120	GLU	N-CA-C	5.63	117.79	109.69
1	C	122	TYR	N-CA-C	-5.63	101.52	109.96
1	B	176	SER	N-CA-C	-5.61	106.61	113.50
1	C	163	GLY	N-CA-C	5.57	117.25	111.95
1	D	87	PRO	N-CA-C	-5.48	103.24	111.57
1	A	12	CYS	CA-CB-SG	-5.47	101.82	114.40
1	D	118	MET	N-CA-C	-5.47	99.15	110.80
1	C	24	ALA	N-CA-C	5.38	117.16	109.14
1	A	8	ALA	N-CA-C	5.35	117.11	111.28
1	A	108	THR	N-CA-C	-5.31	107.81	114.56
1	C	180	LEU	N-CA-C	5.18	117.41	109.07
1	B	55	ILE	N-CA-C	5.13	116.20	109.58
1	D	144	LYS	N-CA-C	-5.13	102.99	110.08
1	D	170	PRO	N-CA-C	-5.11	103.42	111.34
1	C	148	VAL	N-CA-C	-5.10	105.42	110.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1663	0	1638	68	0
1	B	1686	0	1669	35	0
1	C	1655	0	1627	53	0
1	D	1668	0	1645	74	0
2	A	8	0	0	0	0
3	A	64	0	0	1	0
3	B	95	0	0	0	0
3	C	66	0	0	2	0
3	D	78	0	0	1	0
All	All	6983	0	6579	223	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 17.

All (223) 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:1:ARG:H	1:B:56:ASN:HD22	1.08	1.00
1:B:148:VAL:HG12	1:B:152:MET:HE2	1.46	0.98
1:A:1:ARG:HB2	1:A:1:ARG:HH11	1.26	0.97
1:A:1:ARG:H	1:A:56:ASN:HD22	1.13	0.95
1:D:1:ARG:H	1:D:56:ASN:HD22	1.14	0.95
1:D:64:PRO:O	1:D:93:THR:HG21	1.69	0.92
1:D:148:VAL:HG12	1:D:152:MET:HE2	1.55	0.88
1:D:174:LYS:O	1:D:175:GLU:HG2	1.71	0.88
1:A:117:ARG:HH11	1:A:120:GLU:HG3	1.37	0.87
1:C:62:ARG:HD3	1:C:215:VAL:HB	1.60	0.84
1:D:149:HIS:HA	1:D:152:MET:HE3	1.60	0.83
1:C:147:ILE:HD12	3:C:2045:HOH:O	1.83	0.79
1:A:171:ASP:HA	1:A:174:LYS:HD3	1.64	0.79
1:A:25:HIS:HB3	1:A:40:MET:HE2	1.63	0.79
1:D:63:GLY:C	1:D:93:THR:HG22	2.11	0.76
1:A:51:SER:OG	1:A:53:THR:HG22	1.85	0.75
1:A:42:GLN:HE22	1:B:210:GLU:HB3	1.50	0.75
1:B:111:LEU:HD13	1:B:159:TRP:CE3	2.21	0.75
1:C:123:TRP:HB3	1:C:143:LEU:HD21	1.68	0.75
1:D:1:ARG:H	1:D:56:ASN:ND2	1.84	0.75
1:B:1:ARG:H	1:B:56:ASN:ND2	1.86	0.74
1:D:31:ARG:HG2	1:D:33:HIS:H	1.52	0.73
1:C:152:MET:HE1	1:C:172:LEU:O	1.88	0.73
1:C:143:LEU:N	1:C:143:LEU:HD23	2.02	0.73
1:C:171:ASP:HA	1:C:174:LYS:HD3	1.71	0.72
1:D:158:GLU:HB3	1:D:181:ARG:NH2	2.04	0.72
1:A:148:VAL:HG12	1:A:152:MET:HE2	1.70	0.72
1:A:38:LEU:O	1:A:42:GLN:HG3	1.91	0.71
1:A:1:ARG:HH12	1:A:56:ASN:HD21	1.39	0.70
1:D:18:ASN:C	1:D:18:ASN:HD22	1.97	0.70
1:D:111:LEU:HD13	1:D:159:TRP:CE3	2.25	0.70
1:A:198:CYS:HB3	3:A:2055:HOH:O	1.92	0.69
1:D:31:ARG:H	1:D:31:ARG:HD2	1.56	0.68
1:A:170:PRO:HG3	1:D:24:ALA:O	1.93	0.68
1:D:152:MET:HE1	1:D:173:GLY:HA2	1.74	0.68
1:D:31:ARG:HG3	1:D:33:HIS:CG	2.30	0.66
1:B:151:ARG:HH11	1:B:154:GLN:NE2	1.94	0.66
1:B:62:ARG:HG2	1:B:91:VAL:O	1.96	0.65
1:D:27:GLU:OE1	1:D:36:ARG:NH1	2.30	0.65
1:A:1:ARG:HH12	1:A:56:ASN:ND2	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:THR:HG23	1:D:109:ARG:HG3	1.79	0.65
1:A:117:ARG:NH1	1:A:120:GLU:HG3	2.09	0.64
1:A:111:LEU:HD13	1:A:159:TRP:CE3	2.32	0.64
1:D:120:GLU:HG2	1:D:144:LYS:HD2	1.79	0.64
1:D:129:ASP:OD2	1:D:133:ILE:HG23	1.98	0.64
1:D:38:LEU:HB2	1:D:39:PRO:HD3	1.80	0.63
1:D:130:GLU:CD	1:D:130:GLU:H	2.07	0.63
1:D:117:ARG:HG2	1:D:117:ARG:HH11	1.63	0.62
1:D:12:CYS:CB	1:D:29:CYS:SG	2.88	0.61
1:C:62:ARG:CD	1:C:215:VAL:HB	2.28	0.61
1:C:111:LEU:HD13	1:C:159:TRP:CE3	2.35	0.61
1:A:36:ARG:O	1:A:40:MET:HG3	2.00	0.61
1:A:1:ARG:H	1:A:56:ASN:ND2	1.93	0.61
1:A:29:CYS:HB3	1:A:33:HIS:O	2.01	0.61
1:A:94:LEU:HD13	1:A:124:ALA:HB2	1.82	0.60
1:B:160:VAL:HA	1:B:181:ARG:O	2.02	0.60
1:A:84:ALA:O	1:A:86:LEU:HD13	2.01	0.60
1:C:117:ARG:CA	1:C:117:ARG:HH11	2.14	0.60
1:A:170:PRO:O	1:A:174:LYS:HE2	2.01	0.59
1:A:0:LEU:HD23	1:A:1:ARG:N	2.17	0.59
1:A:194:LEU:HB2	1:A:195:PRO:HD3	1.84	0.59
1:D:63:GLY:O	1:D:93:THR:HG22	2.03	0.59
1:A:210:GLU:HB2	1:B:39:PRO:HG3	1.84	0.58
1:B:111:LEU:HG	1:B:123:TRP:CH2	2.38	0.58
1:D:194:LEU:HB2	1:D:195:PRO:HD3	1.83	0.58
1:A:1:ARG:HH11	1:A:1:ARG:CB	2.08	0.58
1:D:31:ARG:HG3	1:D:33:HIS:ND1	2.19	0.58
1:D:75:GLY:HA2	1:D:78:GLN:HE21	1.68	0.58
1:A:148:VAL:O	1:A:152:MET:HG3	2.04	0.58
1:D:0:LEU:HD22	1:D:2:ILE:HG13	1.85	0.58
1:B:151:ARG:HH11	1:B:154:GLN:HE21	1.50	0.57
1:C:62:ARG:O	1:C:62:ARG:HG2	2.05	0.57
1:A:82:LEU:C	1:A:82:LEU:HD23	2.30	0.56
1:A:152:MET:HE1	1:A:172:LEU:O	2.04	0.56
1:A:7:THR:O	1:A:33:HIS:HE1	1.89	0.56
1:A:152:MET:O	1:A:178:LEU:HD11	2.06	0.56
1:C:117:ARG:HH11	1:C:117:ARG:CB	2.20	0.55
1:D:18:ASN:C	1:D:18:ASN:ND2	2.64	0.55
1:B:1:ARG:N	1:B:56:ASN:HD22	1.92	0.55
1:A:1:ARG:HB2	1:A:1:ARG:NH1	2.10	0.54
1:D:107:ALA:HB1	1:D:160:VAL:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:THR:HB	1:A:166:TRP:CE2	2.43	0.54
1:A:171:ASP:HA	1:A:174:LYS:CD	2.36	0.54
1:D:152:MET:CE	1:D:173:GLY:HA2	2.38	0.54
1:D:-2:ALA:N	3:D:2001:HOH:O	2.40	0.54
1:B:143:LEU:HD13	1:B:148:VAL:CG2	2.38	0.54
1:A:1:ARG:NH1	1:A:56:ASN:ND2	2.55	0.53
1:B:152:MET:HE1	1:B:172:LEU:O	2.09	0.53
1:C:38:LEU:HD13	1:D:78:GLN:HB3	1.89	0.53
1:A:36:ARG:C	1:A:39:PRO:HD2	2.33	0.53
1:A:70:VAL:HG13	1:A:71:ARG:N	2.23	0.53
1:A:75:GLY:HA2	1:A:78:GLN:HE21	1.73	0.53
1:B:143:LEU:HD13	1:B:148:VAL:HG22	1.91	0.53
1:C:143:LEU:N	1:C:143:LEU:CD2	2.71	0.53
1:C:123:TRP:O	1:C:140:GLU:HA	2.09	0.53
1:A:121:VAL:HG12	1:A:143:LEU:O	2.09	0.52
1:D:114:ILE:HB	1:D:122:TYR:HB2	1.92	0.52
1:A:42:GLN:NE2	1:B:210:GLU:HB3	2.24	0.52
1:C:38:LEU:CD1	1:D:78:GLN:HB3	2.40	0.52
1:C:194:LEU:HB2	1:C:195:PRO:HD3	1.92	0.52
1:D:1:ARG:NH1	1:D:18:ASN:HD21	2.09	0.51
1:B:110:VAL:HG22	1:B:160:VAL:CG2	2.41	0.51
1:C:117:ARG:HB3	1:C:117:ARG:NH1	2.24	0.51
1:D:33:HIS:HB3	1:D:35:GLN:HG2	1.92	0.51
1:D:213:GLU:HB2	1:D:214:PRO:HD2	1.90	0.51
1:A:203:GLU:OE1	1:A:205:LYS:HE2	2.10	0.51
1:D:31:ARG:HG2	1:D:33:HIS:N	2.24	0.51
1:C:160:VAL:HA	1:C:181:ARG:O	2.10	0.51
1:A:3:LEU:HB2	1:A:55:ILE:HD13	1.91	0.51
1:C:37:ILE:O	1:C:41:VAL:HG23	2.11	0.51
1:D:137:GLU:O	1:D:140:GLU:HG3	2.10	0.51
1:D:52:LEU:HD12	1:D:55:ILE:HD12	1.93	0.50
1:C:52:LEU:HD23	1:C:55:ILE:HD12	1.93	0.50
1:C:116:ALA:C	1:C:118:MET:H	2.20	0.50
1:C:158:GLU:HG2	1:C:179:VAL:HB	1.91	0.50
1:C:207:VAL:CG2	1:C:211:HIS:HB2	2.40	0.50
1:D:1:ARG:NH1	1:D:18:ASN:ND2	2.60	0.50
1:D:119:GLY:O	1:D:145:PRO:HD3	2.12	0.50
1:C:117:ARG:HH11	1:C:117:ARG:HA	1.76	0.49
1:D:31:ARG:CG	1:D:33:HIS:CG	2.94	0.49
1:D:74:ILE:O	1:D:78:GLN:HG3	2.12	0.49
1:C:51:SER:HB3	1:C:54:ASP:OD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:-1:GLY:HA3	1:C:19:ASP:OD1	2.13	0.49
1:A:6:ASP:O	1:A:12:CYS:HA	2.13	0.48
1:A:169:TRP:C	1:A:171:ASP:H	2.21	0.48
1:C:71:ARG:HG3	1:C:71:ARG:HH11	1.78	0.48
1:D:158:GLU:HB3	1:D:181:ARG:HH21	1.76	0.48
1:A:117:ARG:HG3	1:A:118:MET:H	1.77	0.48
1:B:62:ARG:HG2	1:B:91:VAL:C	2.37	0.48
1:C:146:GLU:O	1:C:149:HIS:HB3	2.13	0.48
1:B:84:ALA:CB	1:B:86:LEU:HD13	2.43	0.48
1:D:1:ARG:HG2	1:D:1:ARG:HH11	1.78	0.48
1:A:117:ARG:HG3	1:A:120:GLU:HB2	1.96	0.48
1:D:31:ARG:HG3	1:D:31:ARG:HH11	1.79	0.48
1:D:160:VAL:HA	1:D:181:ARG:O	2.14	0.48
1:B:84:ALA:HB3	1:B:86:LEU:HD13	1.94	0.48
1:D:158:GLU:HG2	1:D:179:VAL:HB	1.96	0.48
1:B:0:LEU:HD22	1:B:2:ILE:HG13	1.96	0.47
1:D:63:GLY:C	1:D:93:THR:CG2	2.87	0.47
1:A:210:GLU:CB	1:B:39:PRO:HG3	2.44	0.47
1:A:111:LEU:HG	1:A:123:TRP:CH2	2.50	0.47
1:B:94:LEU:HD13	1:B:124:ALA:HB2	1.97	0.47
1:D:116:ALA:O	1:D:118:MET:HG3	2.14	0.47
1:D:51:SER:HB3	1:D:54:ASP:OD2	2.14	0.47
1:D:195:PRO:O	1:D:199:GLN:HG3	2.15	0.47
1:B:36:ARG:C	1:B:39:PRO:HD2	2.39	0.47
1:D:170:PRO:O	1:D:171:ASP:HB2	2.15	0.46
1:A:-1:GLY:HA3	1:A:19:ASP:OD1	2.15	0.46
1:A:94:LEU:HD12	1:A:140:GLU:HG2	1.96	0.46
1:B:-4:LYS:NZ	1:B:-4:LYS:HB3	2.30	0.46
1:D:110:VAL:HG22	1:D:160:VAL:CG2	2.45	0.46
1:C:117:ARG:HH11	1:C:117:ARG:HB3	1.80	0.46
1:A:158:GLU:HB3	1:A:179:VAL:HB	1.97	0.46
1:B:114:ILE:HB	1:B:122:TYR:HB2	1.97	0.46
1:D:12:CYS:SG	1:D:29:CYS:SG	3.13	0.46
1:C:35:GLN:H	1:C:35:GLN:HG3	1.39	0.46
1:D:12:CYS:HB3	1:D:29:CYS:SG	2.57	0.46
1:A:119:GLY:O	1:A:145:PRO:HD3	2.15	0.45
1:B:38:LEU:HD22	1:B:38:LEU:N	2.32	0.45
1:C:166:TRP:CE3	1:C:172:LEU:HD23	2.51	0.45
1:A:12:CYS:SG	1:A:29:CYS:N	2.89	0.45
1:C:23:ASN:ND2	1:C:44:ILE:HG23	2.32	0.45
1:A:82:LEU:HD23	1:A:82:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:LEU:HD22	1:D:159:TRP:CB	2.47	0.45
1:C:89:ILE:HG12	1:C:206:THR:HG22	1.99	0.45
1:C:156:SER:HA	1:C:178:LEU:CD2	2.47	0.45
1:C:52:LEU:HA	1:C:55:ILE:HD12	1.99	0.45
1:C:94:LEU:HD13	1:C:124:ALA:HB2	2.00	0.44
1:A:97:MET:HE1	1:A:114:ILE:HG12	1.99	0.44
1:D:1:ARG:NH1	1:D:19:ASP:OD1	2.50	0.44
1:B:161:THR:HG22	1:B:166:TRP:CZ2	2.52	0.44
1:C:16:LEU:HB2	1:C:44:ILE:HG21	1.99	0.44
1:C:114:ILE:HB	1:C:122:TYR:HB2	1.98	0.44
1:C:18:ASN:O	1:C:19:ASP:HB2	2.18	0.44
1:C:77:ALA:HB1	1:C:88:MET:HE3	1.99	0.44
1:C:158:GLU:HG2	1:C:179:VAL:CB	2.48	0.44
1:D:123:TRP:O	1:D:140:GLU:HA	2.18	0.44
1:D:116:ALA:HB1	1:D:118:MET:HE3	1.99	0.44
1:A:108:THR:O	1:A:127:GLN:HA	2.17	0.44
1:A:209:VAL:HG23	1:A:210:GLU:N	2.33	0.44
1:D:1:ARG:HH11	1:D:18:ASN:ND2	2.15	0.44
1:D:94:LEU:HD13	1:D:124:ALA:HB2	1.99	0.43
1:C:1:ARG:HA	1:C:17:TRP:O	2.19	0.43
1:A:34:THR:HG21	1:A:72:ILE:CG2	2.49	0.43
1:B:194:LEU:HB2	1:B:195:PRO:HD3	2.00	0.43
1:C:36:ARG:HG3	3:C:2015:HOH:O	2.17	0.43
1:D:31:ARG:HG3	1:D:31:ARG:NH1	2.34	0.43
1:A:1:ARG:N	1:A:56:ASN:HD22	1.96	0.43
1:A:7:THR:HG21	1:A:34:THR:HG22	2.01	0.43
1:B:36:ARG:O	1:B:39:PRO:HD2	2.18	0.43
1:C:204:GLY:C	1:C:206:THR:H	2.26	0.43
1:D:86:LEU:HA	1:D:87:PRO:HD3	1.85	0.43
1:D:125:GLU:OE2	1:D:155:LEU:HD11	2.18	0.43
1:A:52:LEU:HD23	1:A:55:ILE:HD12	2.01	0.43
1:B:45:LEU:HD11	1:B:52:LEU:HD13	2.00	0.43
1:C:207:VAL:HG22	1:C:208:ALA:N	2.33	0.43
1:C:56:ASN:O	1:C:87:PRO:HD2	2.18	0.42
1:D:18:ASN:HD22	1:D:19:ASP:N	2.16	0.42
1:D:55:ILE:HG22	1:D:57:ALA:H	1.84	0.42
1:A:7:THR:O	1:A:33:HIS:CE1	2.71	0.42
1:A:22:VAL:HG23	1:A:22:VAL:O	2.20	0.42
1:C:62:ARG:CG	1:C:215:VAL:HB	2.49	0.42
1:A:169:TRP:C	1:A:171:ASP:N	2.76	0.42
1:B:130:GLU:HA	1:B:130:GLU:OE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:TYR:CD2	1:D:88:MET:HE2	2.54	0.42
1:D:111:LEU:HG	1:D:123:TRP:CH2	2.55	0.41
1:A:117:ARG:O	1:A:118:MET:O	2.37	0.41
1:A:55:ILE:O	1:A:86:LEU:HD21	2.20	0.41
1:B:143:LEU:CD1	1:B:148:VAL:HG22	2.50	0.41
1:C:173:GLY:O	1:C:176:SER:HB3	2.20	0.41
1:A:50:THR:HG22	1:A:51:SER:N	2.35	0.41
1:C:109:ARG:HD3	1:C:158:GLU:O	2.21	0.41
1:A:117:ARG:HG3	1:A:118:MET:N	2.35	0.41
1:C:128:ARG:NH1	1:C:132:GLY:HA2	2.35	0.41
1:B:52:LEU:HD12	1:B:52:LEU:HA	1.88	0.41
1:C:124:ALA:HB2	1:C:140:GLU:HG2	2.03	0.41
1:A:213:GLU:HB2	1:A:214:PRO:CD	2.50	0.40
1:C:143:LEU:HD23	1:C:143:LEU:H	1.83	0.40
1:D:117:ARG:HG2	1:D:117:ARG:NH1	2.33	0.40
1:D:33:HIS:C	1:D:35:GLN:N	2.79	0.40
1:D:3:LEU:HB2	1:D:55:ILE:HD13	2.03	0.40
1:C:111:LEU:HG	1:C:123:TRP:CH2	2.56	0.40
1:B:129:ASP:OD1	1:B:129:ASP:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	218/251 (87%)	200 (92%)	14 (6%)	4 (2%)	6	5
1	B	221/251 (88%)	213 (96%)	8 (4%)	0	100	100
1	C	217/251 (86%)	206 (95%)	11 (5%)	0	100	100
1	D	219/251 (87%)	215 (98%)	4 (2%)	0	100	100
All	All	875/1004 (87%)	834 (95%)	37 (4%)	4 (0%)	24	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	ARG
1	A	118	MET
1	A	20	GLY
1	A	106	GLY

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	170/199 (85%)	162 (95%)	8 (5%)	23	33
1	B	172/199 (86%)	163 (95%)	9 (5%)	21	28
1	C	169/199 (85%)	161 (95%)	8 (5%)	23	33
1	D	170/199 (85%)	162 (95%)	8 (5%)	23	33
All	All	681/796 (86%)	648 (95%)	33 (5%)	23	32

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

Mol	Chain	Res	Type
1	A	0	LEU
1	A	1	ARG
1	A	12	CYS
1	A	29	CYS
1	A	58	LEU
1	A	111	LEU
1	A	143	LEU
1	A	217	LEU
1	B	-4	LYS
1	B	0	LEU
1	B	35	GLN
1	B	47	THR
1	B	52	LEU
1	B	111	LEU
1	B	121	VAL
1	B	143	LEU

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Mol	Chain	Res	Type
1	B	209	VAL
1	C	12	CYS
1	C	16	LEU
1	C	35	GLN
1	C	62	ARG
1	C	111	LEU
1	C	117	ARG
1	C	143	LEU
1	C	213	GLU
1	D	0	LEU
1	D	18	ASN
1	D	23	ASN
1	D	36	ARG
1	D	111	LEU
1	D	130	GLU
1	D	133	ILE
1	D	217	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	33	HIS
1	A	42	GLN
1	A	56	ASN
1	A	78	GLN
1	A	127	GLN
1	A	153	GLN
1	A	167	GLN
1	A	199	GLN
1	B	35	GLN
1	B	42	GLN
1	B	56	ASN
1	B	78	GLN
1	B	131	ASN
1	B	149	HIS
1	B	154	GLN
1	B	211	HIS
1	C	18	ASN
1	C	23	ASN
1	C	35	GLN
1	C	78	GLN

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Mol	Chain	Res	Type
1	C	135	HIS
1	C	149	HIS
1	D	18	ASN
1	D	25	HIS
1	D	35	GLN
1	D	56	ASN
1	D	78	GLN
1	D	105	ASN
1	D	127	GLN
1	D	153	GLN
1	D	167	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 8 ligands modelled in this entry, 8 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

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	220/251 (87%)	0.46	13 (5%) 28 29	21, 43, 69, 78	0
1	B	223/251 (88%)	-0.12	3 (1%) 75 76	19, 31, 51, 66	0
1	C	219/251 (87%)	0.23	5 (2%) 61 63	25, 40, 60, 68	0
1	D	221/251 (88%)	0.11	5 (2%) 61 63	22, 35, 54, 69	0
All	All	883/1004 (87%)	0.17	26 (2%) 53 55	19, 37, 62, 78	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	119	GLY	4.9
1	C	118	MET	3.6
1	A	179	VAL	3.5
1	A	118	MET	3.5
1	C	-1	GLY	3.2
1	D	119	GLY	3.1
1	A	19	ASP	3.0
1	A	173	GLY	2.9
1	C	12	CYS	2.9
1	D	175	GLU	2.8
1	A	178	LEU	2.7
1	C	119	GLY	2.7
1	A	180	LEU	2.6
1	B	118	MET	2.5
1	A	12	CYS	2.5
1	A	174	LYS	2.5
1	C	216	TYR	2.4
1	D	29	CYS	2.3
1	A	176	SER	2.3
1	D	31	ARG	2.2
1	A	159	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	169	TRP	2.1
1	B	-3	LYS	2.1
1	A	68	THR	2.1
1	D	12	CYS	2.1
1	B	19	ASP	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](#)

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	GD3	A	1220	1/1	0.83	0.33	62,62,62,62	1
2	GD3	A	1218	1/1	0.85	0.27	57,57,57,57	1
2	GD3	A	1213	1/1	0.85	0.36	41,41,41,41	1
2	GD3	A	1215	1/1	0.87	0.32	44,44,44,44	1
2	GD3	A	1216	1/1	0.87	0.27	38,38,38,38	1
2	GD3	A	1217	1/1	0.90	0.45	34,34,34,34	1
2	GD3	A	1219	1/1	0.96	0.51	35,35,35,35	1
2	GD3	A	1214	1/1	0.98	0.24	16,16,16,16	1

6.5 Other polymers [i](#)

There are no such residues in this entry.