



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:55 PM UTC

PDB ID : 2BON / pdb_00002bon
Title : Structure of an Escherichia coli lipid kinase (YegS)
Authors : Bakali, H.M.; Johnson, K.A.; Hallberg, B.M.; Herman, M.D.; Nordlund, P.
Deposited on : 2005-04-12
Resolution : 1.90 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
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

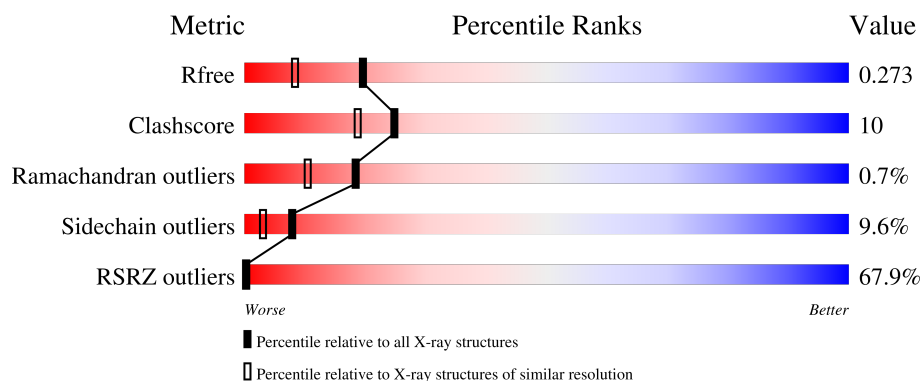
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	332	59% 68% 17% • 14%
1	B	332	54% 58% 19% • 20%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4215 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 LIPID KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2149	1349	374	414	12			
1	B	265	Total	C	N	O	S	0	0	0
			1993	1254	350	377	12			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	expression tag	UNP P76407
A	-23	HIS	-	expression tag	UNP P76407
A	-22	HIS	-	expression tag	UNP P76407
A	-21	HIS	-	expression tag	UNP P76407
A	-20	HIS	-	expression tag	UNP P76407
A	-19	HIS	-	expression tag	UNP P76407
A	-18	HIS	-	expression tag	UNP P76407
A	-17	GLY	-	expression tag	UNP P76407
A	-16	SER	-	expression tag	UNP P76407
A	-15	THR	-	expression tag	UNP P76407
A	-14	SER	-	expression tag	UNP P76407
A	-13	LEU	-	expression tag	UNP P76407
A	-12	TYR	-	expression tag	UNP P76407
A	-11	LYS	-	expression tag	UNP P76407
A	-10	LYS	-	expression tag	UNP P76407
A	-9	ALA	-	expression tag	UNP P76407
A	-8	GLY	-	expression tag	UNP P76407
A	-7	SER	-	expression tag	UNP P76407
A	-6	GLU	-	expression tag	UNP P76407
A	-5	THR	-	expression tag	UNP P76407
A	-4	LEU	-	expression tag	UNP P76407
A	-3	TYR	-	expression tag	UNP P76407
A	-2	ILE	-	expression tag	UNP P76407
A	-1	GLN	-	expression tag	UNP P76407
A	0	GLY	-	expression tag	UNP P76407

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Chain	Residue	Modelled	Actual	Comment	Reference
A	300	SER	-	expression tag	UNP P76407
A	301	THR	-	expression tag	UNP P76407
A	302	HIS	-	expression tag	UNP P76407
A	303	HIS	-	expression tag	UNP P76407
A	304	HIS	-	expression tag	UNP P76407
A	305	HIS	-	expression tag	UNP P76407
A	306	HIS	-	expression tag	UNP P76407
A	307	HIS	-	expression tag	UNP P76407
B	-24	MET	-	expression tag	UNP P76407
B	-23	HIS	-	expression tag	UNP P76407
B	-22	HIS	-	expression tag	UNP P76407
B	-21	HIS	-	expression tag	UNP P76407
B	-20	HIS	-	expression tag	UNP P76407
B	-19	HIS	-	expression tag	UNP P76407
B	-18	HIS	-	expression tag	UNP P76407
B	-17	GLY	-	expression tag	UNP P76407
B	-16	SER	-	expression tag	UNP P76407
B	-15	THR	-	expression tag	UNP P76407
B	-14	SER	-	expression tag	UNP P76407
B	-13	LEU	-	expression tag	UNP P76407
B	-12	TYR	-	expression tag	UNP P76407
B	-11	LYS	-	expression tag	UNP P76407
B	-10	LYS	-	expression tag	UNP P76407
B	-9	ALA	-	expression tag	UNP P76407
B	-8	GLY	-	expression tag	UNP P76407
B	-7	SER	-	expression tag	UNP P76407
B	-6	GLU	-	expression tag	UNP P76407
B	-5	THR	-	expression tag	UNP P76407
B	-4	LEU	-	expression tag	UNP P76407
B	-3	TYR	-	expression tag	UNP P76407
B	-2	ILE	-	expression tag	UNP P76407
B	-1	GLN	-	expression tag	UNP P76407
B	0	GLY	-	expression tag	UNP P76407
B	300	SER	-	expression tag	UNP P76407
B	301	THR	-	expression tag	UNP P76407
B	302	HIS	-	expression tag	UNP P76407
B	303	HIS	-	expression tag	UNP P76407
B	304	HIS	-	expression tag	UNP P76407
B	305	HIS	-	expression tag	UNP P76407
B	306	HIS	-	expression tag	UNP P76407
B	307	HIS	-	expression tag	UNP P76407

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

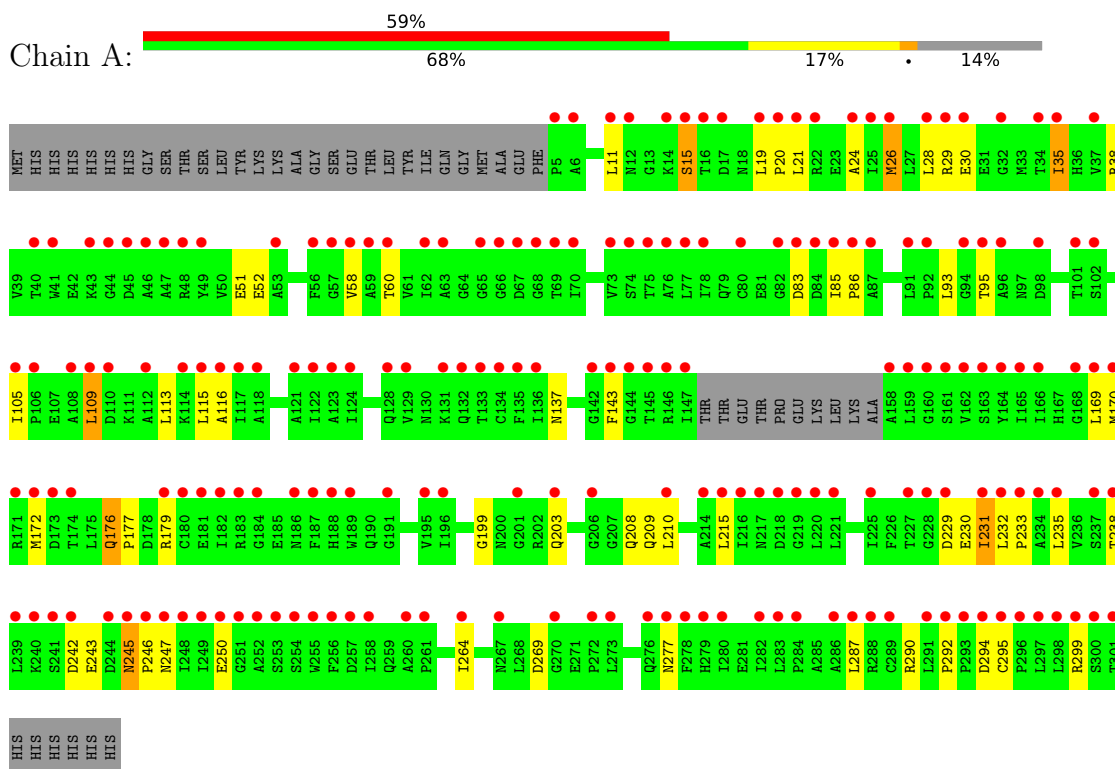
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total 30	O 30	0	0
3	B	41	Total 41	O 41	0	0

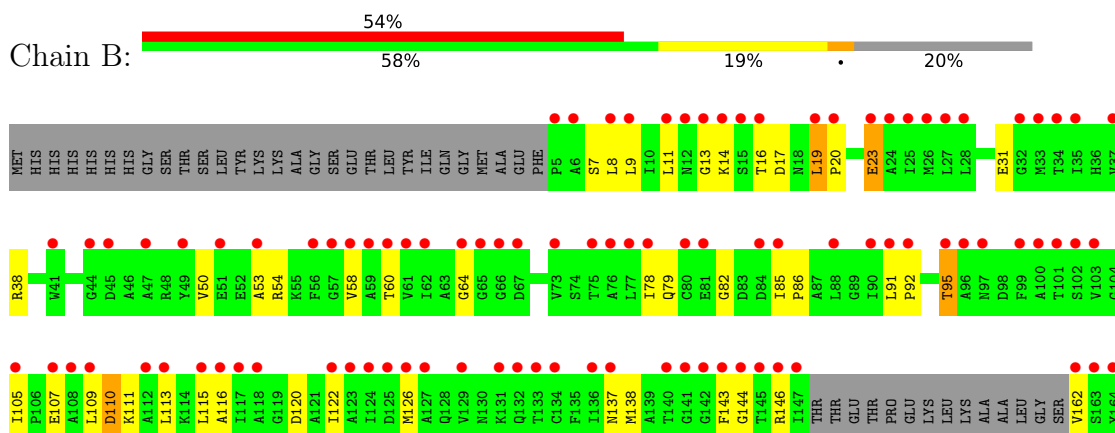
3 Residue-property plots

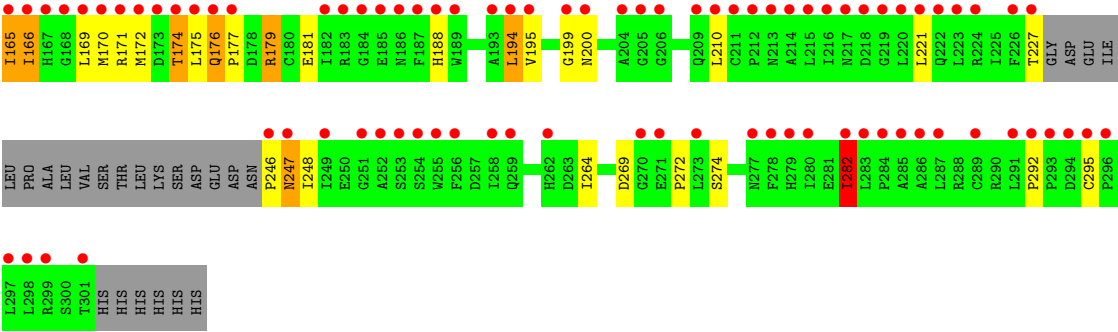
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: LIPID KINASE



• Molecule 1: LIPID KINASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.33Å 166.16Å 48.47Å 90.00° 97.03° 90.00°	Depositor
Resolution (Å)	83.04 – 1.90 83.04 – 1.90	Depositor EDS
% Data completeness (in resolution range)	73.4 (83.04-1.90) 73.4 (83.04-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.220 , 0.267 0.227 , 0.273	Depositor DCC
R_{free} test set	1984 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	1.276	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 74.9	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	0.91	EDS
Total number of atoms	4215	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% 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: MG

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	0.97	4/2184 (0.2%)	1.06	4/2964 (0.1%)
1	B	0.91	0/2026	1.05	5/2746 (0.2%)
All	All	0.94	4/4210 (0.1%)	1.06	9/5710 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	ALA	C-N	10.45	1.46	1.33
1	A	24	ALA	C-O	8.34	1.33	1.24
1	A	26	MET	CG-SD	6.26	1.96	1.80
1	A	26	MET	SD-CE	5.81	1.94	1.79

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	295	CYS	CA-C-N	6.47	126.16	119.56
1	B	295	CYS	C-N-CA	6.47	126.16	119.56
1	A	245	ASN	CA-C-N	6.45	126.95	119.47
1	A	245	ASN	C-N-CA	6.45	126.95	119.47
1	B	199	GLY	N-CA-C	5.98	119.86	110.71
1	A	199	GLY	N-CA-C	5.96	119.83	110.71
1	B	200	ASN	N-CA-C	-5.91	103.53	112.04
1	B	282	ILE	CG1-CB-CG2	-5.86	93.12	110.70
1	A	24	ALA	O-C-N	5.32	127.57	122.03

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	2149	0	2148	38	0
1	B	1993	0	1996	43	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	30	0	0	2	0
3	B	41	0	0	2	0
All	All	4215	0	4144	81	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 10.

All (81) 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:A:176:GLN:HG3	1:A:177:PRO:HD2	1.36	1.08
1:A:170:MET:HB3	1:A:172:MET:HE3	1.47	0.95
1:A:231:ILE:HD12	1:A:231:ILE:H	1.34	0.89
1:B:9:LEU:CD2	1:B:11:LEU:HG	2.07	0.84
1:B:54:ARG:HH12	1:B:82:GLY:HA3	1.46	0.81
1:B:246:PRO:HG2	1:B:248:ILE:HG13	1.64	0.80
1:B:146:ARG:NH1	1:B:272:PRO:HB2	2.00	0.77
1:B:176:GLN:HG3	1:B:177:PRO:HD2	1.67	0.75
1:A:176:GLN:HG3	1:A:177:PRO:CD	2.16	0.73
1:B:169:LEU:HD11	1:B:210:LEU:HD11	1.69	0.73
1:A:26:MET:HB3	3:A:2001:HOH:O	1.88	0.72
1:A:245:ASN:ND2	1:A:247:ASN:H	1.87	0.71
1:A:231:ILE:HD12	1:A:231:ILE:N	2.05	0.70
1:B:115:LEU:HD21	1:B:292:PRO:HD3	1.74	0.69
1:B:143:PHE:CE2	1:B:264:ILE:HG12	2.27	0.69
1:A:38:ARG:HH22	1:A:52:GLU:CD	2.01	0.67
1:A:231:ILE:H	1:A:231:ILE:CD1	2.07	0.67
1:A:38:ARG:NH2	1:A:52:GLU:OE2	2.30	0.65
1:A:28:LEU:HD12	1:A:113:LEU:HD13	1.79	0.63
1:B:221:LEU:HG	1:B:282:ILE:HD12	1.80	0.62
1:B:92:PRO:HD3	1:B:105:ILE:HG21	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ARG:HD3	3:A:2016:HOH:O	2.00	0.61
1:A:35:ILE:O	1:A:35:ILE:HG13	2.00	0.60
1:B:176:GLN:HG3	1:B:177:PRO:CD	2.31	0.60
1:B:179:ARG:HD3	3:B:2024:HOH:O	2.01	0.59
1:B:170:MET:HB3	1:B:172:MET:HE3	1.84	0.59
1:A:169:LEU:HD11	1:A:210:LEU:HD11	1.85	0.58
1:B:247:ASN:N	1:B:247:ASN:OD1	2.36	0.58
1:B:179:ARG:CD	3:B:2024:HOH:O	2.53	0.57
1:B:9:LEU:HD22	1:B:11:LEU:HG	1.86	0.54
1:A:245:ASN:C	1:A:245:ASN:HD22	2.16	0.54
1:B:8:LEU:HD11	1:B:38:ARG:HG2	1.89	0.54
1:A:232:LEU:HB3	1:A:233:PRO:HD2	1.89	0.53
1:B:176:GLN:CG	1:B:177:PRO:HD2	2.36	0.53
1:A:116:ALA:O	1:A:290:ARG:HD2	2.09	0.53
1:B:14:LYS:C	1:B:16:THR:H	2.17	0.52
1:A:235:LEU:HA	1:A:238:THR:HG22	1.90	0.52
1:B:9:LEU:HD21	1:B:11:LEU:HG	1.92	0.52
1:B:181:GLU:OE2	1:B:188:HIS:HE1	1.93	0.52
1:B:19:LEU:O	1:B:23:GLU:HG2	2.10	0.51
1:A:137:ASN:HB3	1:A:269:ASP:OD1	2.12	0.50
1:A:11:LEU:HD22	1:A:15:SER:CB	2.42	0.49
1:B:143:PHE:CZ	1:B:264:ILE:HG12	2.47	0.49
1:B:165:ILE:O	1:B:169:LEU:HB3	2.11	0.49
1:B:144:GLY:HA3	1:B:174:THR:HG22	1.94	0.49
1:A:208:GLN:HE21	1:A:208:GLN:HA	1.78	0.49
1:A:38:ARG:NH2	1:A:52:GLU:CD	2.70	0.47
1:A:60:THR:HG21	1:A:116:ALA:O	2.15	0.47
1:B:19:LEU:N	1:B:20:PRO:HD2	2.30	0.47
1:A:143:PHE:CE2	1:A:264:ILE:HG12	2.50	0.46
1:A:215:LEU:HD13	1:A:299:ARG:HB3	1.98	0.46
1:B:50:VAL:O	1:B:53:ALA:HB3	2.16	0.46
1:B:14:LYS:C	1:B:16:THR:N	2.73	0.46
1:B:110:ASP:C	1:B:110:ASP:OD2	2.58	0.46
1:A:245:ASN:HD22	1:A:246:PRO:N	2.14	0.46
1:A:245:ASN:ND2	1:A:245:ASN:C	2.73	0.46
1:A:21:LEU:HD13	1:A:93:LEU:HD11	1.99	0.45
1:B:146:ARG:NH2	1:B:274:SER:OG	2.50	0.45
1:A:85:ILE:HA	1:A:86:PRO:HD3	1.92	0.44
1:A:60:THR:HG1	1:A:290:ARG:HE	1.66	0.44
1:B:165:ILE:O	1:B:170:MET:HG2	2.18	0.43
1:B:92:PRO:HD3	1:B:105:ILE:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:THR:HG21	1:B:116:ALA:O	2.19	0.43
1:B:166:ILE:O	1:B:170:MET:HB2	2.19	0.43
1:A:38:ARG:HD3	1:A:38:ARG:HA	1.79	0.42
1:B:8:LEU:HD22	1:B:53:ALA:HB2	2.01	0.42
1:B:138:MET:HE2	1:B:138:MET:HB2	1.82	0.42
1:A:26:MET:O	1:A:30:GLU:HG2	2.18	0.42
1:A:238:THR:HA	1:A:243:GLU:HB2	2.02	0.42
1:A:203:GLN:OE1	1:A:209:GLN:NE2	2.52	0.42
1:A:294:ASP:O	1:A:295:CYS:C	2.63	0.42
1:B:194:LEU:HD23	1:B:195:VAL:HG23	2.01	0.42
1:B:14:LYS:HE2	1:B:17:ASP:OD2	2.20	0.41
1:A:109:LEU:H	1:A:109:LEU:HD12	1.84	0.41
1:B:64:GLY:HA2	1:B:91:LEU:HB2	2.02	0.41
1:B:8:LEU:CD2	1:B:53:ALA:HB2	2.50	0.41
1:B:111:LYS:HD2	1:B:111:LYS:HA	1.85	0.41
1:A:115:LEU:HD21	1:A:292:PRO:HD3	2.02	0.41
1:B:85:ILE:HA	1:B:86:PRO:HD3	1.95	0.40
1:B:137:ASN:HB3	1:B:269:ASP:OD1	2.21	0.40
1:A:19:LEU:HB3	1:A:20:PRO:HD3	2.02	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	283/332 (85%)	268 (95%)	13 (5%)	2 (1%)	18	10
1	B	259/332 (78%)	244 (94%)	13 (5%)	2 (1%)	16	8
All	All	542/664 (82%)	512 (94%)	26 (5%)	4 (1%)	18	10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	13	GLY
1	A	15	SER
1	A	229	ASP
1	B	95	THR

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	228/267 (85%)	213 (93%)	15 (7%)	15	8
1	B	210/267 (79%)	183 (87%)	27 (13%)	4	1
All	All	438/534 (82%)	396 (90%)	42 (10%)	8	3

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	35	ILE
1	A	51	GLU
1	A	58	VAL
1	A	83	ASP
1	A	95	THR
1	A	105	ILE
1	A	109	LEU
1	A	176	GLN
1	A	230	GLU
1	A	231	ILE
1	A	242	ASP
1	A	250	GLU
1	A	277	ASN
1	A	287	LEU
1	B	7	SER
1	B	19	LEU
1	B	23	GLU
1	B	31	GLU
1	B	58	VAL

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Mol	Chain	Res	Type
1	B	78	ILE
1	B	79	GLN
1	B	95	THR
1	B	107	GLU
1	B	109	LEU
1	B	110	ASP
1	B	113	LEU
1	B	120	ASP
1	B	122	ILE
1	B	126	MET
1	B	162	VAL
1	B	165	ILE
1	B	166	ILE
1	B	171	ARG
1	B	174	THR
1	B	175	LEU
1	B	176	GLN
1	B	179	ARG
1	B	194	LEU
1	B	227	THR
1	B	247	ASN
1	B	282	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	GLN
1	A	203	GLN
1	A	208	GLN
1	A	209	GLN
1	A	222	GLN
1	A	245	ASN
1	B	188	HIS
1	B	190	GLN
1	B	259	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](#)

Of 2 ligands modelled in this entry, 2 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 [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	287/332 (86%)	2.58	196 (68%)  	45, 65, 76, 88	0
1	B	265/332 (79%)	2.62	179 (67%)  	57, 65, 81, 95	0
All	All	552/664 (83%)	2.60	375 (67%)  	45, 65, 79, 95	0

All (375) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	166	ILE	6.5
1	A	78	ILE	6.4
1	A	25	ILE	6.2
1	B	255	TRP	6.1
1	B	147	ILE	6.0
1	A	108	ALA	6.0
1	B	184	GLY	5.6
1	B	65	GLY	5.6
1	A	255	TRP	5.3
1	B	165	ILE	5.3
1	A	123	ALA	5.3
1	B	25	ILE	5.2
1	A	286	ALA	5.2
1	A	301	THR	5.1
1	B	167	HIS	5.1
1	B	32	GLY	5.1
1	B	144	GLY	5.0
1	B	168	GLY	5.0
1	A	238	THR	4.9
1	B	174	THR	4.9
1	B	164	TYR	4.9
1	A	63	ALA	4.9
1	B	285	ALA	4.8
1	B	217	ASN	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	234	ALA	4.8
1	B	282	ILE	4.7
1	B	27	LEU	4.7
1	B	170	MET	4.7
1	B	177	PRO	4.6
1	B	246	PRO	4.6
1	B	284	PRO	4.6
1	B	220	LEU	4.6
1	B	162	VAL	4.5
1	A	24	ALA	4.5
1	A	246	PRO	4.5
1	B	215	LEU	4.5
1	B	187	PHE	4.4
1	B	112	ALA	4.4
1	A	37	VAL	4.3
1	A	284	PRO	4.3
1	A	160	GLY	4.3
1	A	96	ALA	4.3
1	A	300	SER	4.2
1	A	112	ALA	4.2
1	A	158	ALA	4.2
1	A	293	PRO	4.2
1	B	56	PHE	4.1
1	B	64	GLY	4.1
1	A	232	LEU	4.1
1	B	13	GLY	4.1
1	B	16	THR	4.1
1	B	101	THR	4.1
1	B	77	LEU	4.1
1	A	162	VAL	4.1
1	A	83	ASP	4.1
1	A	147	ILE	4.0
1	B	78	ILE	4.0
1	A	186	ASN	4.0
1	A	115	LEU	4.0
1	B	194	LEU	4.0
1	B	19	LEU	4.0
1	A	184	GLY	4.0
1	A	292	PRO	3.9
1	B	37	VAL	3.9
1	B	254	SER	3.9
1	B	145	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	124	ILE	3.9
1	B	199	GLY	3.8
1	A	163	SER	3.8
1	B	133	THR	3.8
1	B	115	LEU	3.8
1	A	15	SER	3.8
1	A	254	SER	3.8
1	A	82	GLY	3.7
1	A	239	LEU	3.7
1	A	16	THR	3.7
1	B	186	ASN	3.7
1	B	283	LEU	3.7
1	B	108	ALA	3.7
1	B	146	ARG	3.7
1	B	169	LEU	3.7
1	A	46	ALA	3.7
1	B	256	PHE	3.7
1	A	145	THR	3.7
1	A	85	ILE	3.6
1	A	299	ARG	3.6
1	A	28	LEU	3.6
1	A	220	LEU	3.6
1	B	58	VAL	3.6
1	B	172	MET	3.6
1	A	53	ALA	3.5
1	B	109	LEU	3.6
1	A	166	ILE	3.5
1	A	248	ILE	3.5
1	A	253	SER	3.5
1	B	293	PRO	3.5
1	A	252	ALA	3.5
1	A	260	ALA	3.5
1	A	287	LEU	3.5
1	A	228	GLY	3.5
1	A	188	HIS	3.5
1	A	233	PRO	3.5
1	B	95	THR	3.5
1	B	117	ILE	3.5
1	A	282	ILE	3.5
1	B	193	ALA	3.5
1	B	249	ILE	3.4
1	B	57	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	116	ALA	3.4
1	A	297	LEU	3.4
1	A	132	GLN	3.4
1	B	124	ILE	3.4
1	A	187	PHE	3.4
1	B	183	ARG	3.4
1	A	70	ILE	3.3
1	A	58	VAL	3.3
1	A	47	ALA	3.3
1	B	47	ALA	3.3
1	B	218	ASP	3.3
1	A	183	ARG	3.3
1	A	235	LEU	3.3
1	A	278	PHE	3.3
1	A	29	ARG	3.3
1	B	134	CYS	3.3
1	A	231	ILE	3.3
1	A	244	ASP	3.3
1	B	205	GLY	3.3
1	B	15	SER	3.3
1	A	118	ALA	3.2
1	A	121	ALA	3.2
1	B	286	ALA	3.2
1	A	129	VAL	3.2
1	B	175	LEU	3.2
1	B	80	CYS	3.2
1	A	164	TYR	3.2
1	B	212	PRO	3.2
1	A	215	LEU	3.2
1	B	210	LEU	3.2
1	B	143	PHE	3.2
1	B	24	ALA	3.2
1	A	86	PRO	3.2
1	B	20	PRO	3.2
1	B	296	PRO	3.2
1	A	206	GLY	3.2
1	B	81	GLU	3.2
1	A	214	ALA	3.1
1	A	172	MET	3.1
1	A	56	PHE	3.1
1	B	222	GLN	3.1
1	A	76	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	53	ALA	3.1
1	A	182	ILE	3.1
1	B	219	GLY	3.1
1	A	257	ASP	3.1
1	A	95	THR	3.1
1	B	92	PRO	3.1
1	B	252	ALA	3.1
1	B	182	ILE	3.1
1	A	109	LEU	3.1
1	A	189	TRP	3.1
1	B	221	LEU	3.1
1	A	75	THR	3.1
1	A	174	THR	3.1
1	A	227	THR	3.1
1	B	75	THR	3.1
1	A	168	GLY	3.1
1	B	6	ALA	3.1
1	A	45	ASP	3.0
1	A	258	ILE	3.0
1	B	67	ASP	3.0
1	B	291	LEU	3.0
1	B	279	HIS	3.0
1	B	163	SER	3.0
1	A	6	ALA	3.0
1	B	216	ILE	3.0
1	B	280	ILE	3.0
1	B	11	LEU	3.0
1	A	34	THR	3.0
1	B	60	THR	3.0
1	A	94	GLY	3.0
1	A	249	ILE	3.0
1	A	291	LEU	3.0
1	A	40	THR	3.0
1	A	44	GLY	3.0
1	A	68	GLY	3.0
1	B	289	CYS	3.0
1	B	35	ILE	3.0
1	A	77	LEU	2.9
1	B	34	THR	2.9
1	B	227	THR	2.9
1	A	87	ALA	2.9
1	B	123	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	298	LEU	2.9
1	A	142	GLY	2.9
1	B	301	THR	2.9
1	A	245	ASN	2.9
1	A	135	PHE	2.9
1	A	273	LEU	2.9
1	A	283	LEU	2.9
1	A	217	ASN	2.9
1	A	279	HIS	2.9
1	B	188	HIS	2.9
1	A	289	CYS	2.9
1	A	74	SER	2.9
1	B	84	ASP	2.9
1	A	298	LEU	2.9
1	B	88	LEU	2.9
1	A	133	THR	2.8
1	A	106	PRO	2.8
1	B	292	PRO	2.8
1	A	256	PHE	2.8
1	B	100	ALA	2.8
1	B	295	CYS	2.8
1	A	26	MET	2.8
1	A	196	ILE	2.8
1	B	9	LEU	2.8
1	B	28	LEU	2.8
1	A	32	GLY	2.8
1	A	219	GLY	2.8
1	B	132	GLN	2.8
1	A	295	CYS	2.8
1	B	287	LEU	2.8
1	B	61	VAL	2.8
1	A	180	CYS	2.8
1	A	277	ASN	2.8
1	B	297	LEU	2.8
1	B	173	ASP	2.8
1	A	241	SER	2.7
1	A	247	ASN	2.7
1	B	214	ALA	2.7
1	B	278	PHE	2.7
1	B	251	GLY	2.7
1	B	122	ILE	2.7
1	B	126	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	146	ARG	2.7
1	B	195	VAL	2.7
1	B	271	GLU	2.7
1	A	136	ILE	2.7
1	B	62	ILE	2.7
1	A	237	SER	2.7
1	B	299	ARG	2.7
1	A	131	LYS	2.7
1	A	57	GLY	2.7
1	A	20	PRO	2.7
1	A	261	PRO	2.7
1	B	91	LEU	2.7
1	A	98	ASP	2.6
1	A	14	LYS	2.6
1	A	240	LYS	2.6
1	B	253	SER	2.6
1	B	258	ILE	2.6
1	A	66	GLY	2.6
1	A	73	VAL	2.6
1	A	229	ASP	2.6
1	A	242	ASP	2.6
1	B	118	ALA	2.6
1	A	105	ILE	2.6
1	A	264	ILE	2.6
1	B	85	ILE	2.6
1	B	66	GLY	2.6
1	B	59	ALA	2.6
1	A	114	LYS	2.6
1	B	14	LYS	2.6
1	A	12	ASN	2.6
1	A	272	PRO	2.6
1	B	176	GLN	2.6
1	B	294	ASP	2.6
1	A	116	ALA	2.6
1	B	127	ALA	2.6
1	B	277	ASN	2.6
1	B	49	TYR	2.5
1	B	171	ARG	2.5
1	B	259	GLN	2.5
1	A	67	ASP	2.5
1	A	280	ILE	2.5
1	B	90	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	105	ILE	2.5
1	A	181	GLU	2.5
1	A	17	ASP	2.5
1	B	125	ASP	2.5
1	A	159	LEU	2.5
1	B	8	LEU	2.5
1	A	117	ILE	2.5
1	A	122	ILE	2.5
1	B	189	TRP	2.5
1	B	137	ASN	2.5
1	B	96	ALA	2.5
1	B	204	ALA	2.5
1	B	33	MET	2.5
1	B	73	VAL	2.5
1	B	200	ASN	2.5
1	B	247	ASN	2.5
1	A	102	SER	2.5
1	A	161	SER	2.5
1	A	173	ASP	2.5
1	B	12	ASN	2.4
1	B	213	ASN	2.4
1	A	165	ILE	2.4
1	A	101	THR	2.4
1	B	141	GLY	2.4
1	B	113	LEU	2.4
1	B	136	ILE	2.4
1	B	262	HIS	2.4
1	B	270	GLY	2.4
1	A	134	CYS	2.4
1	A	11	LEU	2.4
1	A	144	GLY	2.4
1	A	195	VAL	2.4
1	B	211	CYS	2.4
1	A	19	LEU	2.3
1	A	143	PHE	2.3
1	A	60	THR	2.3
1	B	140	THR	2.3
1	A	267	ASN	2.3
1	A	296	PRO	2.3
1	B	5	PRO	2.3
1	A	221	LEU	2.3
1	A	69	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	76	ALA	2.3
1	A	84	ASP	2.3
1	A	62	ILE	2.3
1	A	250	GLU	2.3
1	A	80	CYS	2.3
1	A	21	LEU	2.3
1	B	273	LEU	2.3
1	A	110	ASP	2.2
1	A	294	ASP	2.2
1	B	209	GLN	2.2
1	A	288	ARG	2.2
1	A	91	LEU	2.2
1	B	185	GLU	2.2
1	A	128	GLN	2.2
1	B	44	GLY	2.2
1	A	59	ALA	2.2
1	B	99	PHE	2.2
1	A	179	ARG	2.2
1	A	169	LEU	2.2
1	A	218	ASP	2.2
1	B	142	GLY	2.2
1	A	5	PRO	2.2
1	A	270	GLY	2.2
1	B	223	LEU	2.2
1	A	43	LYS	2.2
1	A	171	ARG	2.2
1	B	45	ASP	2.1
1	A	201	GLY	2.1
1	B	206	GLY	2.1
1	B	226	PHE	2.1
1	B	41	TRP	2.1
1	B	102	SER	2.1
1	B	26	MET	2.1
1	A	210	LEU	2.1
1	A	203	GLN	2.1
1	A	49	TYR	2.1
1	A	225	ILE	2.1
1	A	22	ARG	2.1
1	A	48	ARG	2.1
1	B	23	GLU	2.1
1	A	191	GLY	2.1
1	B	97	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	129	VAL	2.1
1	A	65	GLY	2.0
1	A	41	TRP	2.0
1	B	224	ARG	2.0
1	A	30	GLU	2.0
1	B	51	GLU	2.0
1	B	107	GLU	2.0
1	B	131	LYS	2.0
1	A	170	MET	2.0
1	A	35	ILE	2.0
1	A	216	ILE	2.0
1	A	251	GLY	2.0
1	A	276	GLN	2.0
1	A	92	PRO	2.0
1	B	103	VAL	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	MG	B	1302	1/1	0.92	0.15	65,65,65,65	0
2	MG	A	1302	1/1	0.97	0.11	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.