



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 08:29 pm GMT

PDB ID : 2BON  
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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

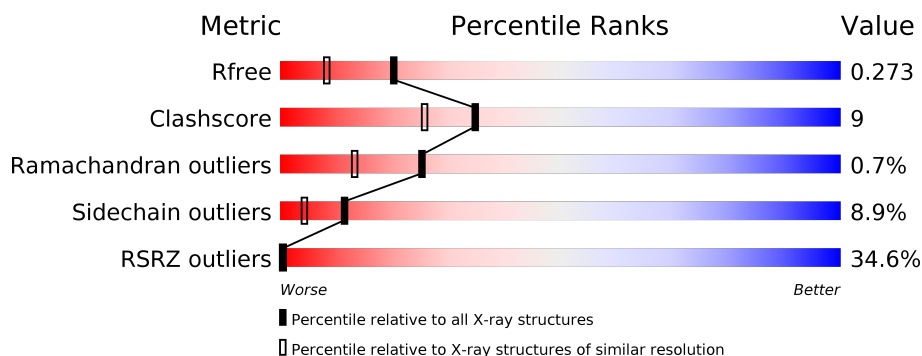
# 1 Overall quality at a glance

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))
$R_{free}$	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	332	<div> <div>30%</div> <div>69% 14% • 14%</div> </div>
1	B	332	<div> <div>28%</div> <div>58% 18% • • 20%</div> </div>

## 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 (three-letter code: MG) (formula: Mg).

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

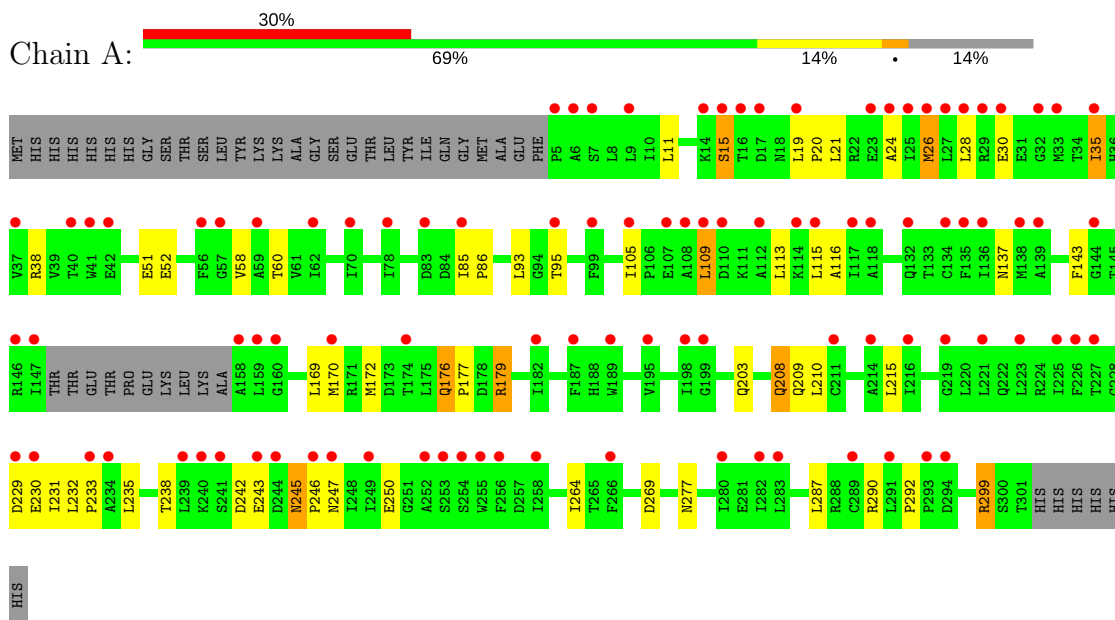
- Molecule 3 is water.

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

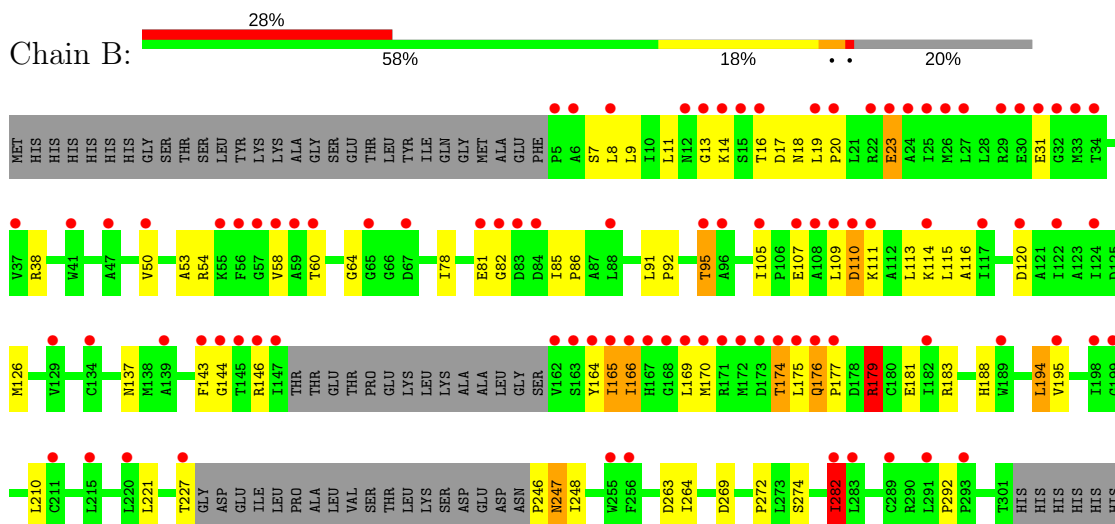
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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, $\alpha$ , $\beta$ , $\gamma$	42.33Å 166.16Å 48.47Å 90.00° 97.03° 90.00°	Depositor
Resolution (Å)	83.04 – 1.90 42.01 – 1.90	Depositor EDS
% Data completeness (in resolution range)	73.4 (83.04-1.90) 73.4 (42.01-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.47%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.1	Xtriage
Anisotropy	1.276	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 85.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4215	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.74	3/2184 (0.1%)	0.82	2/2964 (0.1%)
1	B	0.72	0/2026	0.82	4/2746 (0.1%)
All	All	0.73	3/4210 (0.1%)	0.82	6/5710 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	MET	CG-SD	5.87	1.96	1.81
1	A	24	ALA	C-N	5.54	1.46	1.34
1	A	24	ALA	C-O	5.43	1.33	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	282	ILE	CG1-CB-CG2	-8.31	93.12	111.40
1	A	299	ARG	NE-CZ-NH1	-6.51	117.04	120.30
1	A	179	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	B	263	ASP	CB-CG-OD1	5.09	122.88	118.30
1	B	179	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	183	ARG	NE-CZ-NH1	5.02	122.81	120.30

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	36	0
1	B	1993	0	1996	42	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	78	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 9.

All (78) 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:231:ILE:H	1:A:231:ILE:HD12	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:231:ILE:H	1:A:231:ILE:CD1	2.07	0.67
1:A:170:MET:HB3	1:A:172:MET:HE2	1.76	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:A:38:ARG:HH22	1:A:52:GLU:CD	2.01	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
1:A:179:ARG:HD3	3:A:2016:HOH:O	2.00	0.61
1:A:35:ILE:HG13	1:A:35:ILE:O	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:HE2	1:B:175:LEU:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:LEU:HD11	1:A:210:LEU:HD11	1.85	0.58
1:A:170:MET:HB3	1:A:172:MET:CE	2.34	0.58
1:B:247:ASN:OD1	1:B:247:ASN:N	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: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: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:165:ILE:O	1:B:169:LEU:HB3	2.11	0.49
1:B:143:PHE:CZ	1:B:264:ILE:HG12	2.47	0.49
1:B:144:GLY:HA3	1:B:174:THR:HG22	1.94	0.49
1:A:208:GLN:HA	1:A:208:GLN:HE21	1.78	0.49
1:A:245:ASN:HD22	1:A:245:ASN:C	2.16	0.48
1:B:14:LYS:C	1:B:16:THR:H	2.17	0.48
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:A:245:ASN:HD22	1:A:246:PRO:N	2.14	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: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
1:B:166:ILE:O	1:B:170:MET:HB2	2.19	0.43
1:B:60:THR:HG21	1:B:116:ALA:O	2.19	0.43
1:A:38:ARG:HA	1:A:38:ARG:HD3	1.79	0.42
1:B:8:LEU:HD22	1:B:53:ALA:HB2	2.01	0.42
1:A:26:MET:O	1:A:30:GLU:HG2	2.18	0.42
1:B:110:ASP:C	1:B:110:ASP:OD2	2.58	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:B:194:LEU:HD23	1:B:195:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:LYS:HE2	1:B:17:ASP:OD2	2.20	0.41
1:A:109:LEU:HD12	1:A:109:LEU:H	1.84	0.41
1:A:245:ASN:ND2	1:A:245:ASN:C	2.73	0.41
1:B:14:LYS:C	1:B:16:THR:N	2.73	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:HA	1:B:111:LYS:HD2	1.85	0.41
1:A:115:LEU:HD21	1:A:292:PRO:HD3	2.02	0.41
1:B:137:ASN:HB3	1:B:269:ASP:OD1	2.21	0.40
1:B:85:ILE:HA	1:B:86:PRO:HD3	1.95	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

### 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	283/332 (85%)	268 (95%)	13 (5%)	2 (1%)	25	13
1	B	259/332 (78%)	244 (94%)	13 (5%)	2 (1%)	22	11
All	All	542/664 (82%)	512 (94%)	26 (5%)	4 (1%)	25	13

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%)	214 (94%)	14 (6%)	22	11
1	B	210/267 (79%)	185 (88%)	25 (12%)	6	2
All	All	438/534 (82%)	399 (91%)	39 (9%)	11	4

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	51	GLU
1	A	58	VAL
1	A	95	THR
1	A	105	ILE
1	A	109	LEU
1	A	176	GLN
1	A	208	GLN
1	A	230	GLU
1	A	242	ASP
1	A	245	ASN
1	A	250	GLU
1	A	277	ASN
1	A	287	LEU
1	B	7	SER
1	B	18	ASN
1	B	23	GLU
1	B	31	GLU
1	B	58	VAL
1	B	78	ILE
1	B	81	GLU
1	B	95	THR
1	B	107	GLU
1	B	109	LEU
1	B	110	ASP
1	B	113	LEU
1	B	114	LYS

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Mol	Chain	Res	Type
1	B	120	ASP
1	B	126	MET
1	B	164	TYR
1	B	165	ILE
1	B	166	ILE
1	B	174	THR
1	B	176	GLN
1	B	179	ARG
1	B	194	LEU
1	B	227	THR
1	B	247	ASN
1	B	282	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) 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	245	ASN
1	B	18	ASN
1	B	188	HIS
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 ⓘ

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

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	287/332 (86%)	1.89	99 (34%) <b>0</b> <b>0</b>	45, 65, 76, 88	0
1	B	265/332 (79%)	2.04	92 (34%) <b>0</b> <b>0</b>	57, 65, 81, 95	0
All	All	552/664 (83%)	1.96	191 (34%) <b>0</b> <b>0</b>	45, 65, 79, 95	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	164	TYR	12.4
1	A	16	THR	11.8
1	B	147	ILE	10.4
1	B	162	VAL	10.2
1	B	117	ILE	8.4
1	B	166	ILE	8.3
1	B	146	ARG	8.2
1	A	28	LEU	7.4
1	B	169	LEU	7.1
1	B	167	HIS	7.0
1	B	27	LEU	6.9
1	A	30	GLU	6.9
1	B	16	THR	6.7
1	B	175	LEU	6.5
1	A	158	ALA	6.3
1	B	170	MET	6.2
1	A	26	MET	6.1
1	A	108	ALA	5.8
1	A	147	ILE	5.8
1	B	83	ASP	5.8
1	A	146	ARG	5.6
1	A	243	GLU	5.5
1	A	109	LEU	5.5
1	B	32	GLY	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	241	SER	5.5
1	B	173	ASP	5.5
1	B	25	ILE	5.4
1	A	27	LEU	5.2
1	B	172	MET	5.2
1	B	165	ILE	5.1
1	B	33	MET	5.0
1	B	110	ASP	5.0
1	A	240	LYS	4.9
1	B	171	ARG	4.9
1	B	109	LEU	4.8
1	B	58	VAL	4.8
1	B	174	THR	4.8
1	B	163	SER	4.7
1	A	118	ALA	4.7
1	B	13	GLY	4.7
1	B	144	GLY	4.7
1	B	30	GLU	4.6
1	B	65	GLY	4.6
1	A	105	ILE	4.4
1	A	57	GLY	4.4
1	A	174	THR	4.4
1	B	26	MET	4.3
1	B	145	THR	4.3
1	B	84	ASP	4.3
1	A	33	MET	4.1
1	B	34	THR	4.1
1	B	168	GLY	4.1
1	A	19	LEU	4.0
1	A	14	LYS	3.9
1	A	59	ALA	3.8
1	B	82	GLY	3.8
1	A	293	PRO	3.8
1	A	139	ALA	3.7
1	B	107	GLU	3.7
1	A	15	SER	3.7
1	A	5	PRO	3.6
1	B	15	SER	3.6
1	A	294	ASP	3.6
1	A	83	ASP	3.6
1	B	81	GLU	3.5
1	A	247	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	229	ASP	3.3
1	B	96	ALA	3.3
1	A	17	ASP	3.3
1	B	67	ASP	3.3
1	A	37	VAL	3.3
1	A	136	ILE	3.2
1	B	19	LEU	3.2
1	B	291	LEU	3.1
1	A	25	ILE	3.1
1	A	252	ALA	3.1
1	B	57	GLY	3.1
1	B	37	VAL	3.1
1	A	24	ALA	3.1
1	A	42	GLU	3.0
1	A	144	GLY	3.0
1	B	177	PRO	3.0
1	B	143	PHE	3.0
1	A	223	LEU	3.0
1	A	114	LYS	3.0
1	A	244	ASP	3.0
1	A	78	ILE	2.9
1	A	85	ILE	2.9
1	A	32	GLY	2.9
1	B	8	LEU	2.9
1	B	282	ILE	2.9
1	A	195	VAL	2.8
1	A	117	ILE	2.8
1	A	56	PHE	2.8
1	B	5	PRO	2.8
1	B	176	GLN	2.8
1	B	105	ILE	2.8
1	A	216	ILE	2.7
1	B	20	PRO	2.7
1	B	55	LYS	2.7
1	A	35	ILE	2.7
1	A	198	ILE	2.7
1	B	227	THR	2.7
1	A	211	CYS	2.7
1	A	138	MET	2.7
1	A	41	TRP	2.7
1	B	12	ASN	2.6
1	A	135	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	214	ALA	2.6
1	B	41	TRP	2.6
1	A	29	ARG	2.6
1	A	226	PHE	2.5
1	A	233	PRO	2.5
1	B	23	GLU	2.5
1	A	258	ILE	2.5
1	A	221	LEU	2.5
1	A	107	GLU	2.5
1	B	6	ALA	2.5
1	A	112	ALA	2.5
1	A	115	LEU	2.5
1	A	159	LEU	2.5
1	A	7	SER	2.5
1	B	59	ALA	2.4
1	B	50	VAL	2.4
1	A	187	PHE	2.4
1	B	293	PRO	2.4
1	A	282	ILE	2.4
1	B	24	ALA	2.4
1	B	60	THR	2.4
1	B	29	ARG	2.4
1	B	124	ILE	2.4
1	B	195	VAL	2.4
1	B	283	LEU	2.4
1	A	110	ASP	2.4
1	A	254	SER	2.3
1	B	139	ALA	2.3
1	A	256	PHE	2.3
1	A	134	CYS	2.3
1	A	234	ALA	2.3
1	A	227	THR	2.3
1	B	56	PHE	2.3
1	A	170	MET	2.3
1	A	255	TRP	2.3
1	A	182	ILE	2.3
1	A	230	GLU	2.3
1	A	266	PHE	2.2
1	A	132	GLN	2.2
1	B	108	ALA	2.2
1	B	114	LYS	2.2
1	B	88	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	134	CYS	2.2
1	A	280	ILE	2.2
1	B	220	LEU	2.2
1	A	246	PRO	2.2
1	B	256	PHE	2.2
1	A	199	GLY	2.2
1	A	62	ILE	2.2
1	B	122	ILE	2.2
1	A	189	TRP	2.2
1	A	283	LEU	2.2
1	B	189	TRP	2.2
1	A	40	THR	2.2
1	B	95	THR	2.2
1	B	47	ALA	2.2
1	B	215	LEU	2.2
1	B	199	GLY	2.2
1	A	99	PHE	2.2
1	A	160	GLY	2.1
1	B	111	LYS	2.1
1	B	255	TRP	2.1
1	A	23	GLU	2.1
1	A	253	SER	2.1
1	A	95	THR	2.1
1	A	291	LEU	2.1
1	B	22	ARG	2.1
1	B	289	CYS	2.1
1	B	14	LYS	2.1
1	B	31	GLU	2.1
1	A	225	ILE	2.1
1	B	198	ILE	2.1
1	A	9	LEU	2.1
1	A	239	LEU	2.1
1	B	129	VAL	2.0
1	A	219	GLY	2.0
1	A	70	ILE	2.0
1	A	249	ILE	2.0
1	A	289	CYS	2.0
1	B	211	CYS	2.0
1	A	6	ALA	2.0
1	B	120	ASP	2.0
1	B	182	ILE	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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	A	1302	1/1	0.91	0.19	-0.85	66,66,66,66	0
2	MG	B	1302	1/1	0.95	0.16	-1.11	65,65,65,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.