



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:46 AM 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.

---

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

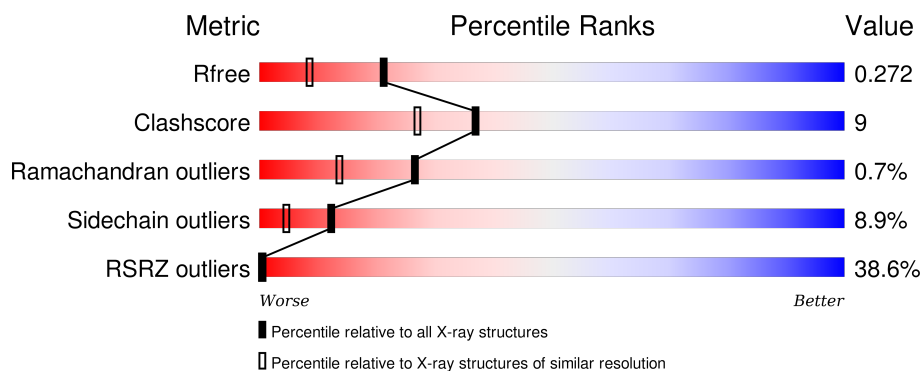
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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>34%</div> <div>69%</div> <div>14%</div> <div>•</div> <div>14%</div> </div>
1	B	332	<div> <div>30%</div> <div>58%</div> <div>18%</div> <div>• •</div> <div>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

*Continued on next page...*

*Continued from previous page...*

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



SIH  
SIH  
SIH  
SIH  
SIH  
SIH  
SIH

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.33 Å 166.16 Å 48.47 Å 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 1.89 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.220 , 0.267 0.227 , 0.272	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 , 85.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 38253 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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

*Continued on next page...*

*Continued from previous page...*

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:B:176:GLN:CG	1:B:177:PRO:HD2	2.36	0.53
1:A:232:LEU:HB3	1:A:233:PRO:HD2	1.89	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: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:A:11:LEU:HD22	1:A:15:SER:CB	2.42	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

*Continued on next page...*

Continued from previous page...

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: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:A:109:LEU:HD12	1:A:109:LEU:H	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: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: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

### 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%)	26	14
1	B	259/332 (78%)	244 (94%)	13 (5%)	2 (1%)	24	11
All	All	542/664 (82%)	512 (94%)	26 (5%)	4 (1%)	26	14

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%)	23	11
1	B	210/267 (79%)	185 (88%)	25 (12%)	6	2
All	All	438/534 (82%)	399 (91%)	39 (9%)	12	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

*Continued on next page...*

*Continued from previous page...*

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%)	1.99	114 (39%) <b>0</b> <b>0</b>	45, 65, 76, 88	0
1	B	265/332 (79%)	2.14	99 (37%) <b>0</b> <b>0</b>	57, 65, 81, 95	0
All	All	552/664 (83%)	2.06	213 (38%) <b>0</b> <b>0</b>	45, 65, 79, 95	0

All (213) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	164	TYR	13.3
1	A	16	THR	11.9
1	B	147	ILE	10.6
1	B	162	VAL	10.4
1	B	117	ILE	9.2
1	B	166	ILE	8.5
1	B	146	ARG	8.1
1	A	28	LEU	7.6
1	B	169	LEU	7.4
1	B	27	LEU	7.3
1	B	167	HIS	7.2
1	B	16	THR	7.1
1	A	158	ALA	6.9
1	A	30	GLU	6.9
1	B	175	LEU	6.8
1	B	170	MET	6.5
1	A	108	ALA	6.4
1	A	26	MET	6.1
1	A	241	SER	5.9
1	B	25	ILE	5.9
1	B	83	ASP	5.7
1	A	147	ILE	5.7
1	B	32	GLY	5.7
1	B	165	ILE	5.7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	146	ARG	5.6
1	A	109	LEU	5.6
1	B	173	ASP	5.5
1	A	243	GLU	5.5
1	A	27	LEU	5.4
1	B	110	ASP	5.1
1	B	33	MET	5.1
1	B	13	GLY	5.1
1	A	240	LYS	5.1
1	B	174	THR	4.9
1	B	58	VAL	4.9
1	B	109	LEU	4.9
1	B	172	MET	4.9
1	B	144	GLY	4.9
1	B	171	ARG	4.8
1	A	118	ALA	4.8
1	B	163	SER	4.8
1	B	30	GLU	4.8
1	B	84	ASP	4.7
1	B	65	GLY	4.6
1	A	174	THR	4.6
1	A	105	ILE	4.6
1	B	145	THR	4.5
1	A	57	GLY	4.4
1	B	26	MET	4.4
1	B	168	GLY	4.2
1	A	19	LEU	4.1
1	A	14	LYS	4.1
1	B	34	THR	4.1
1	A	293	PRO	4.1
1	A	59	ALA	4.1
1	A	33	MET	4.0
1	A	139	ALA	3.9
1	B	107	GLU	3.9
1	A	15	SER	3.8
1	B	82	GLY	3.8
1	A	83	ASP	3.7
1	B	15	SER	3.7
1	A	294	ASP	3.7
1	A	5	PRO	3.7
1	B	81	GLU	3.6
1	A	247	ASN	3.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	96	ALA	3.4
1	A	229	ASP	3.4
1	A	25	ILE	3.4
1	A	17	ASP	3.4
1	B	19	LEU	3.4
1	B	291	LEU	3.4
1	A	136	ILE	3.3
1	B	67	ASP	3.3
1	A	244	ASP	3.3
1	A	85	ILE	3.3
1	A	37	VAL	3.2
1	A	78	ILE	3.2
1	A	24	ALA	3.2
1	A	252	ALA	3.2
1	B	37	VAL	3.2
1	A	114	LYS	3.2
1	A	117	ILE	3.1
1	B	143	PHE	3.1
1	A	42	GLU	3.1
1	A	144	GLY	3.1
1	B	177	PRO	3.1
1	B	57	GLY	3.1
1	A	223	LEU	3.1
1	A	56	PHE	3.0
1	A	32	GLY	3.0
1	B	20	PRO	3.0
1	B	282	ILE	3.0
1	A	195	VAL	2.9
1	A	35	ILE	2.9
1	B	105	ILE	2.9
1	A	216	ILE	2.9
1	B	50	VAL	2.9
1	B	176	GLN	2.8
1	B	12	ASN	2.8
1	B	55	LYS	2.8
1	B	8	LEU	2.8
1	A	198	ILE	2.8
1	B	5	PRO	2.8
1	B	227	THR	2.8
1	A	159	LEU	2.8
1	A	41	TRP	2.8
1	A	211	CYS	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	135	PHE	2.7
1	A	115	LEU	2.7
1	A	258	ILE	2.7
1	A	138	MET	2.7
1	A	214	ALA	2.7
1	A	221	LEU	2.7
1	B	41	TRP	2.7
1	A	233	PRO	2.6
1	A	226	PHE	2.6
1	A	29	ARG	2.6
1	B	23	GLU	2.6
1	A	112	ALA	2.6
1	A	107	GLU	2.6
1	A	187	PHE	2.6
1	B	60	THR	2.6
1	B	56	PHE	2.6
1	A	234	ALA	2.6
1	B	6	ALA	2.6
1	B	59	ALA	2.6
1	A	110	ASP	2.6
1	A	282	ILE	2.5
1	B	124	ILE	2.5
1	B	195	VAL	2.5
1	B	24	ALA	2.5
1	B	293	PRO	2.5
1	A	7	SER	2.5
1	B	88	LEU	2.5
1	A	134	CYS	2.4
1	A	132	GLN	2.4
1	B	139	ALA	2.4
1	B	29	ARG	2.4
1	A	170	MET	2.4
1	B	283	LEU	2.4
1	A	254	SER	2.4
1	A	182	ILE	2.4
1	A	256	PHE	2.4
1	A	266	PHE	2.4
1	B	108	ALA	2.4
1	A	280	ILE	2.4
1	A	227	THR	2.4
1	B	256	PHE	2.4
1	A	62	ILE	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	255	TRP	2.3
1	B	134	CYS	2.3
1	B	47	ALA	2.3
1	B	122	ILE	2.3
1	B	220	LEU	2.3
1	B	189	TRP	2.3
1	A	40	THR	2.3
1	B	215	LEU	2.3
1	A	160	GLY	2.3
1	A	230	GLU	2.3
1	A	189	TRP	2.3
1	A	283	LEU	2.3
1	B	114	LYS	2.3
1	A	199	GLY	2.3
1	B	199	GLY	2.3
1	A	291	LEU	2.2
1	A	246	PRO	2.2
1	A	99	PHE	2.2
1	A	239	LEU	2.2
1	B	14	LYS	2.2
1	B	255	TRP	2.2
1	A	23	GLU	2.2
1	B	211	CYS	2.2
1	A	253	SER	2.2
1	B	198	ILE	2.2
1	B	95	THR	2.2
1	A	50	VAL	2.2
1	A	70	ILE	2.2
1	A	225	ILE	2.2
1	A	249	ILE	2.2
1	B	287	LEU	2.2
1	B	111	LYS	2.2
1	A	204	ALA	2.1
1	B	182	ILE	2.1
1	A	95	THR	2.1
1	A	6	ALA	2.1
1	A	76	ALA	2.1
1	B	129	VAL	2.1
1	B	22	ARG	2.1
1	A	289	CYS	2.1
1	B	289	CYS	2.1
1	A	232	LEU	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	20	PRO	2.1
1	A	219	GLY	2.1
1	B	187	PHE	2.1
1	B	226	PHE	2.1
1	A	9	LEU	2.1
1	A	220	LEU	2.1
1	A	207	GLY	2.1
1	B	135	PHE	2.1
1	A	215	LEU	2.1
1	B	180	CYS	2.1
1	A	100	ALA	2.0
1	A	231	ILE	2.0
1	A	58	VAL	2.0
1	A	140	THR	2.0
1	A	301	THR	2.0
1	B	31	GLU	2.0
1	B	7	SER	2.0
1	A	143	PHE	2.0
1	A	21	LEU	2.0
1	B	221	LEU	2.0
1	B	120	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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(Å <sup>2</sup> )	Q<0.9
2	MG	B	1302	1/1	0.95	0.16	-1.27	65,65,65,65	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	A	1302	1/1	0.91	0.18	-1.28	66,66,66,66	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.