



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:12 PM GMT

PDB ID : 1B9M  
Title : REGULATOR FROM ESCHERICHIA COLI  
Authors : Hall, D.R.; Gourley, D.G.; Hunter, W.N.  
Deposited on : 1999-02-12  
Resolution : 1.75 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

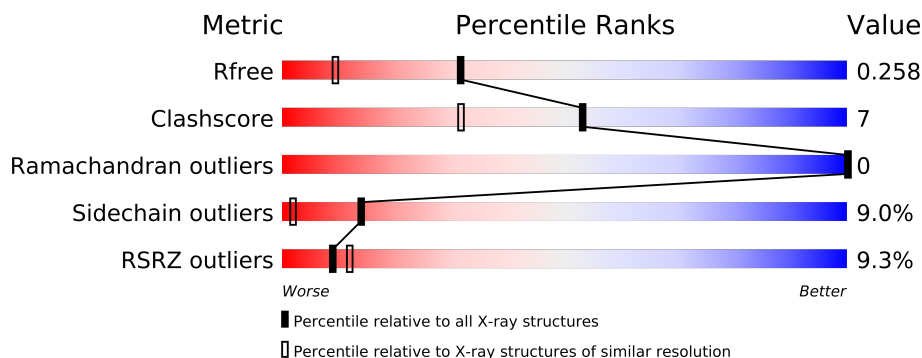
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.75 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))
$R_{free}$	66092	1134 (1.76-1.76)
Clashscore	79885	1304 (1.76-1.76)
Ramachandran outliers	78287	1288 (1.76-1.76)
Sidechain outliers	78261	1288 (1.76-1.76)
RSRZ outliers	66119	1135 (1.76-1.76)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	265	
1	B	265	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4284 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PROTEIN (MODE).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	Se	0	2	0
			1976	1238	350	382	3	3			
1	B	247	Total	C	N	O	S	Se	0	2	0
			1881	1184	326	365	3	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	SEE REMARK 999	UNP P0A9G8
A	-2	SER	-	SEE REMARK 999	UNP P0A9G8
A	-1	HIS	-	SEE REMARK 999	UNP P0A9G8
A	1	MSE	MET	MODIFIED RESIDUE	UNP P0A9G8
A	55	MSE	MET	MODIFIED RESIDUE	UNP P0A9G8
A	221	MSE	MET	MODIFIED RESIDUE	UNP P0A9G8
B	-3	GLY	-	SEE REMARK 999	UNP P0A9G8
B	-2	SER	-	SEE REMARK 999	UNP P0A9G8
B	-1	HIS	-	SEE REMARK 999	UNP P0A9G8
B	1	MSE	MET	MODIFIED RESIDUE	UNP P0A9G8
B	55	MSE	MET	MODIFIED RESIDUE	UNP P0A9G8
B	221	MSE	MET	MODIFIED RESIDUE	UNP P0A9G8

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ni	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	240	Total	O	0	0
			240	240		

*Continued on next page...*

*Continued from previous page...*

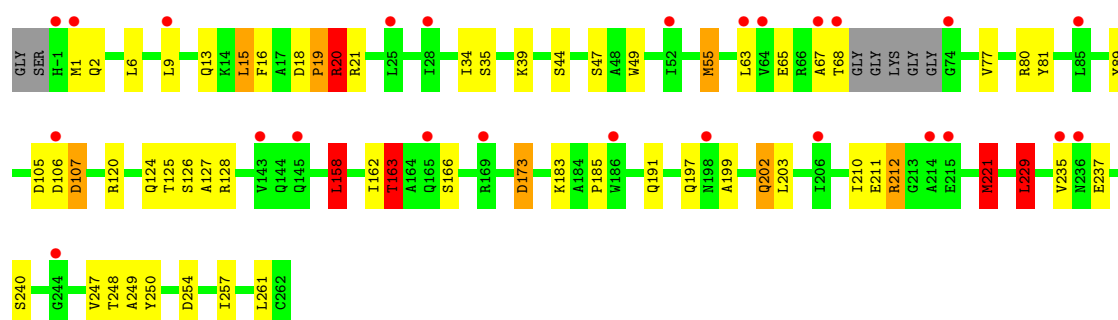
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	186	Total 186	O 186	0	0

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

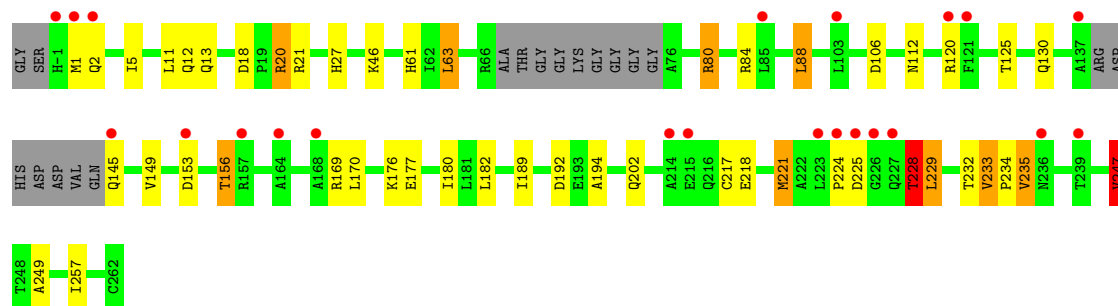
#### • Molecule 1: PROTEIN (MODE)

Chain A: 



#### • Molecule 1: PROTEIN (MODE)

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.61Å 127.24Å 62.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.15 – 1.75 23.21 – 1.75	Depositor EDS
% Data completeness (in resolution range)	80.2 (24.15-1.75) 79.9 (23.21-1.75)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 1.75Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.234 , 0.279 0.221 , 0.258	Depositor DCC
$R_{free}$ test set	2663 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.5	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 54.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 53277 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4284	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI

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	0.78	1/2008 (0.0%)	1.51	29/2717 (1.1%)
1	B	0.66	0/1912	1.43	26/2588 (1.0%)
All	All	0.72	1/3920 (0.0%)	1.47	55/5305 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	MSE	SE-CE	-10.69	1.32	1.95

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20[A]	ARG	CD-NE-CZ	12.08	140.52	123.60
1	A	20[B]	ARG	CD-NE-CZ	12.08	140.52	123.60
1	A	21	ARG	NE-CZ-NH1	11.36	125.98	120.30
1	B	21	ARG	NE-CZ-NH2	11.11	125.85	120.30
1	B	84[A]	ARG	NE-CZ-NH2	-10.20	115.20	120.30
1	B	84[B]	ARG	NE-CZ-NH2	-10.20	115.20	120.30
1	A	20[A]	ARG	NE-CZ-NH2	8.66	124.63	120.30
1	A	20[B]	ARG	NE-CZ-NH2	8.66	124.63	120.30
1	A	80	ARG	NE-CZ-NH2	8.53	124.56	120.30
1	B	84[A]	ARG	NE-CZ-NH1	8.11	124.35	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	84[B]	ARG	NE-CZ-NH1	8.11	124.35	120.30
1	A	212	ARG	CD-NE-CZ	7.95	134.73	123.60
1	A	16	PHE	CB-CG-CD2	-7.70	115.41	120.80
1	B	88	LEU	CA-CB-CG	7.66	132.92	115.30
1	A	163	THR	N-CA-CB	-7.60	95.85	110.30
1	B	229	LEU	CA-CB-CG	7.60	132.77	115.30
1	A	229	LEU	CB-CG-CD1	7.54	123.83	111.00
1	A	65	GLU	OE1-CD-OE2	7.43	132.21	123.30
1	A	21	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	A	80	ARG	NE-CZ-NH1	-7.29	116.65	120.30
1	B	21	ARG	NE-CZ-NH1	-7.20	116.70	120.30
1	B	233	VAL	N-CA-CB	-7.14	95.79	111.50
1	A	250	TYR	CB-CG-CD1	-7.00	116.80	121.00
1	B	247	VAL	N-CA-CB	-6.95	96.20	111.50
1	A	120	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	B	84[A]	ARG	CD-NE-CZ	6.90	133.27	123.60
1	B	84[B]	ARG	CD-NE-CZ	6.90	133.27	123.60
1	A	128	ARG	NE-CZ-NH1	-6.71	116.94	120.30
1	B	235	VAL	CB-CA-C	-6.60	98.86	111.40
1	B	20	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	A	15	LEU	CA-CB-CG	6.54	130.34	115.30
1	B	106	ASP	CB-CG-OD1	6.53	124.17	118.30
1	A	158	LEU	CA-CB-CG	6.35	129.91	115.30
1	A	229	LEU	CA-CB-CG	6.26	129.71	115.30
1	B	233	VAL	CA-CB-CG1	6.16	120.14	110.90
1	A	81	TYR	CB-CG-CD2	-5.97	117.42	121.00
1	A	120	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	B	18	ASP	CB-CG-OD1	5.80	123.52	118.30
1	B	106	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	A	120	ARG	CG-CD-NE	5.51	123.37	111.80
1	B	169	ARG	NE-CZ-NH1	-5.43	117.58	120.30
1	A	126	SER	O-C-N	-5.42	114.03	122.70
1	B	1	MSE	CB-CA-C	-5.42	99.56	110.40
1	A	89	TYR	CG-CD1-CE1	-5.37	117.01	121.30
1	A	221	MSE	CA-CB-CG	5.29	122.29	113.30
1	B	80	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	107	ASP	CA-CB-CG	5.13	124.68	113.40
1	B	13	GLN	O-C-N	-5.10	114.54	122.70
1	A	254	ASP	CB-CG-OD1	-5.08	113.73	118.30
1	B	221	MSE	CA-CB-CG	5.07	121.92	113.30
1	B	88	LEU	CB-CG-CD1	5.06	119.61	111.00
1	A	89	TYR	CB-CG-CD1	-5.06	117.97	121.00

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	228	THR	N-CA-CB	5.05	119.90	110.30
1	A	173	ASP	CA-CB-CG	-5.05	102.29	113.40
1	B	63	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	63	LEU	Mainchain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1976	0	2002	38	0
1	B	1881	0	1895	26	0
2	A	1	0	0	0	0
3	A	240	0	0	2	2
3	B	186	0	0	6	1
All	All	4284	0	3897	54	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (54) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:55:MSE:SE	1:A:55:MSE:CE	1.32	1.51
1:A:55:MSE:HE3	1:A:55:MSE:SE	1.88	1.13
1:A:55:MSE:HE1	1:A:55:MSE:SE	1.88	1.09
1:A:55:MSE:HE2	1:A:55:MSE:SE	1.88	1.08
1:A:221:MSE:HE1	1:A:249:ALA:HB2	1.44	0.97
1:A:221:MSE:HE3	1:A:229:LEU:HG	1.51	0.92
1:A:55:MSE:CG	1:A:55:MSE:CE	2.52	0.86
1:A:163:THR:HG22	1:A:166:SER:H	1.42	0.84
1:B:192:ASP:HB3	3:B:418:HOH:O	1.79	0.83

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:125:THR:H	1:B:130:GLN:HE22	1.30	0.79
1:A:197:GLN:HA	1:A:202:GLN:OE1	1.85	0.75
1:A:20[A]:ARG:HH21	1:A:20[A]:ARG:HB2	1.52	0.74
1:A:158:LEU:HD22	1:A:203:LEU:HD21	1.76	0.67
1:A:124:GLN:HB3	1:B:170:LEU:HD22	1.82	0.61
1:A:125:THR:HB	3:A:456:HOH:O	2.00	0.60
1:A:1:MSE:HE3	1:B:12:GLN:HG3	1.83	0.59
1:B:221:MSE:HE1	1:B:249:ALA:HB2	1.85	0.59
1:A:13:GLN:HE21	1:B:2:GLN:HE22	1.50	0.59
1:B:125:THR:H	1:B:130:GLN:NE2	2.01	0.59
1:A:1:MSE:CE	1:B:11:LEU:HB3	2.35	0.56
1:A:163:THR:CG2	1:A:166:SER:H	2.14	0.56
1:A:257:ILE:HD12	1:B:257:ILE:HD12	1.89	0.55
1:A:125:THR:HG22	1:A:127:ALA:H	1.74	0.53
1:B:27:HIS:HD2	3:B:401:HOH:O	1.92	0.52
1:B:202:GLN:NE2	3:B:411:HOH:O	2.44	0.50
1:A:1:MSE:HE2	1:B:11:LEU:HB3	1.94	0.50
1:B:153:ASP:OD2	1:B:156:THR:HG23	2.11	0.50
1:A:183:LYS:HB3	1:A:185:PRO:HD2	1.94	0.49
1:A:9:LEU:HD22	1:B:5:ILE:HG12	1.95	0.49
1:A:44:SER:OG	1:A:47:SER:HB3	2.14	0.48
1:A:34:ILE:HD12	1:A:49:TRP:CZ2	2.49	0.48
1:A:163:THR:HG22	1:A:166:SER:CB	2.44	0.48
1:B:194:ALA:HB3	3:B:418:HOH:O	2.13	0.47
1:B:218[A]:GLU:OE1	1:B:232:THR:OG1	2.22	0.47
1:A:163:THR:HG22	1:A:166:SER:N	2.21	0.47
1:B:189:ILE:HG23	1:B:247:VAL:HG13	1.96	0.47
1:A:199:ALA:O	1:A:202:GLN:NE2	2.47	0.46
1:A:55:MSE:HE3	1:A:55:MSE:HB2	1.97	0.46
1:A:35:SER:O	1:A:39:LYS:HG3	2.16	0.46
1:B:156:THR:HG22	1:B:224:PRO:HG2	1.98	0.46
1:A:1:MSE:CE	1:B:12:GLN:HG3	2.46	0.45
1:B:228:THR:HB	3:B:440:HOH:O	2.17	0.44
1:A:125:THR:HG22	1:A:127:ALA:N	2.33	0.44
1:A:6:LEU:HD22	1:A:19:PRO:HG2	2.00	0.44
1:A:1:MSE:HE1	1:B:11:LEU:HB3	2.00	0.43
1:B:149:VAL:HG11	1:B:180:ILE:HD11	2.00	0.43
1:A:18:ASP:HB2	1:A:19:PRO:CD	2.48	0.43
1:A:210:ILE:HG22	1:A:211:GLU:N	2.33	0.42
1:A:162:ILE:HG12	1:A:166:SER:HB3	2.01	0.42
3:A:434:HOH:O	1:B:61:HIS:HE1	2.03	0.42
1:A:106:ASP:CG	1:B:80:ARG:HH12	2.23	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:20:ARG:NH2	3:B:290:HOH:O	2.53	0.41
1:B:233:VAL:HA	1:B:234:PRO:HD3	1.93	0.41
1:A:67:ALA:HB2	1:A:77:VAL:HG13	2.02	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:360:HOH:O	3:A:360:HOH:O[2_655]	2.09	0.11
3:A:492:HOH:O	3:B:346:HOH:O[4_456]	2.16	0.04

## 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	256/265 (97%)	249 (97%)	7 (3%)	0	100	100
1	B	243/265 (92%)	239 (98%)	4 (2%)	0	100	100
All	All	499/530 (94%)	488 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	212/210 (101%)	190 (90%)	22 (10%)	10	1
1	B	201/210 (96%)	185 (92%)	16 (8%)	17	2
All	All	413/420 (98%)	375 (91%)	38 (9%)	14	2

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	15	LEU
1	A	19	PRO
1	A	20[A]	ARG
1	A	20[B]	ARG
1	A	68	THR
1	A	105	ASP
1	A	107	ASP
1	A	158	LEU
1	A	163	THR
1	A	173	ASP
1	A	191	GLN
1	A	202	GLN
1	A	212	ARG
1	A	221	MSE
1	A	229	LEU
1	A	235	VAL
1	A	237	GLU
1	A	240	SER
1	A	247	VAL
1	A	248	THR
1	A	261	LEU
1	B	46	LYS
1	B	63	LEU
1	B	88	LEU
1	B	112	ASN
1	B	120	ARG
1	B	145	GLN
1	B	156	THR
1	B	176	LYS
1	B	177	GLU
1	B	182	LEU
1	B	217	CYS
1	B	225	ASP
1	B	228	THR
1	B	229	LEU
1	B	235	VAL
1	B	247	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2	GLN
1	B	94	GLN
1	B	96	GLN
1	B	112	ASN
1	B	130	GLN
1	B	243	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 1 ligands modelled in this entry, 1 is 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.

## 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	258/265 (97%)	0.59	25 (9%) 8 11	26, 35, 64, 87	0
1	B	247/265 (93%)	0.57	22 (8%) 10 13	29, 39, 61, 81	0
All	All	505/530 (95%)	0.58	47 (9%) 9 12	26, 38, 62, 87	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	226	GLY	6.3
1	B	121	PHE	5.7
1	B	-1	HIS	5.5
1	A	74	GLY	5.5
1	B	225	ASP	5.2
1	A	236	ASN	5.2
1	A	214	ALA	5.2
1	B	137	ALA	5.1
1	A	-1	HIS	5.0
1	A	68	THR	4.8
1	B	215	GLU	4.3
1	B	214	ALA	4.2
1	B	223	LEU	3.8
1	A	244	GLY	3.8
1	B	2	GLN	3.7
1	A	143	VAL	3.5
1	B	157	ARG	3.4
1	A	215	GLU	3.4
1	A	206	ILE	3.4
1	B	224	PRO	3.4
1	A	198	ASN	3.2
1	B	227	GLN	3.1
1	B	236	ASN	3.0
1	A	1	MSE	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	85	LEU	3.0
1	B	239	THR	2.6
1	A	165	GLN	2.6
1	A	63	LEU	2.6
1	B	85	LEU	2.5
1	A	106	ASP	2.5
1	A	169	ARG	2.4
1	B	120	ARG	2.4
1	A	186	TRP	2.4
1	B	164	ALA	2.4
1	A	28	ILE	2.3
1	A	235	VAL	2.3
1	B	168	ALA	2.2
1	A	25	LEU	2.2
1	B	145	GLN	2.2
1	A	64	VAL	2.2
1	B	1	MSE	2.1
1	B	103	LEU	2.1
1	A	67	ALA	2.1
1	A	52	ILE	2.1
1	A	145	GLN	2.1
1	A	9	LEU	2.0
1	B	153	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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NI	A	263	1/1	0.04	-3.07	38,38,38,38	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.