



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 23, 2026 – 01:25 PM UTC

PDB ID : 3D71 / pdb\_00003d71  
Title : Crystal structure of E253Q BMRR bound to 22 base pair promoter site  
Authors : Newberry, K.J.; Huffman, J.L.; Brennan, R.G.  
Deposited on : 2008-05-20  
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
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

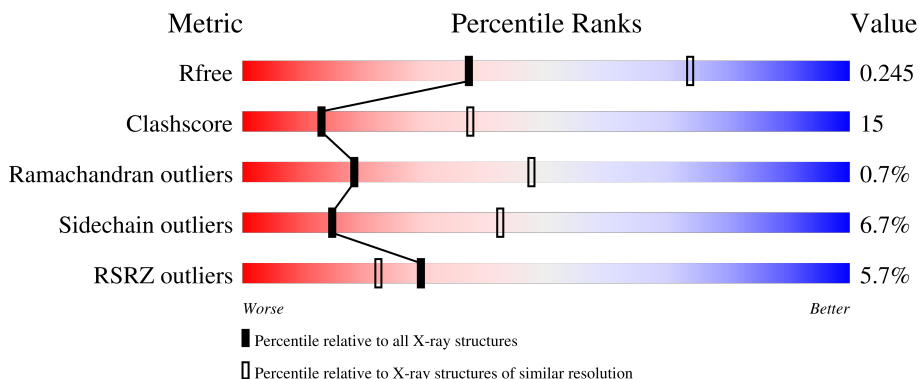
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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  $\geq 3$ , 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	M	24	
2	A	284	

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 2868 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 DNA chain called BMR promoter DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	M	23	468	222	87	137	22	0	0	0

- Molecule 2 is a protein called Multidrug-efflux transporter 1 regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	277	2285	1476	365	436	8	0	0	0

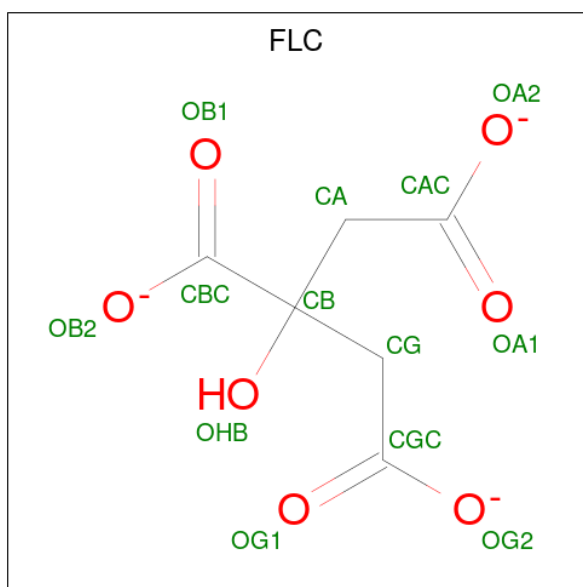
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	253	GLN	GLU	engineered mutation	UNP P39075
A	277	LEU	ALA	engineered mutation	UNP P39075
A	278	ASP	GLU	engineered mutation	UNP P39075
A	279	HIS	-	expression tag	UNP P39075
A	280	HIS	-	expression tag	UNP P39075
A	281	HIS	-	expression tag	UNP P39075
A	282	HIS	-	expression tag	UNP P39075
A	283	HIS	-	expression tag	UNP P39075
A	284	HIS	-	expression tag	UNP P39075

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

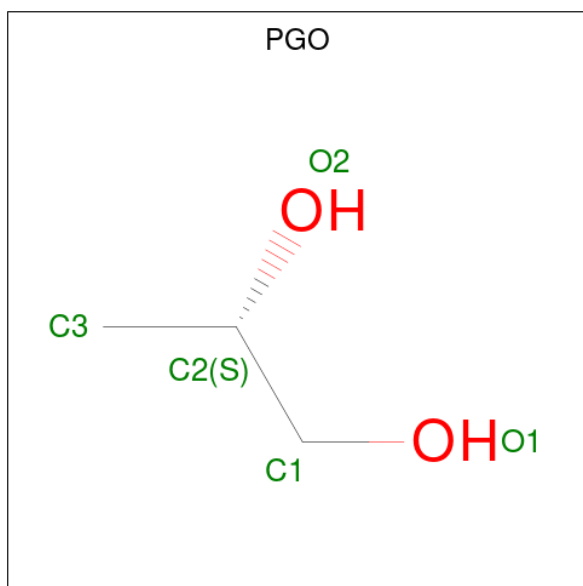
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0

- Molecule 4 is CITRATE ANION (CCD ID: FLC) (formula: C<sub>6</sub>H<sub>5</sub>O<sub>7</sub>).



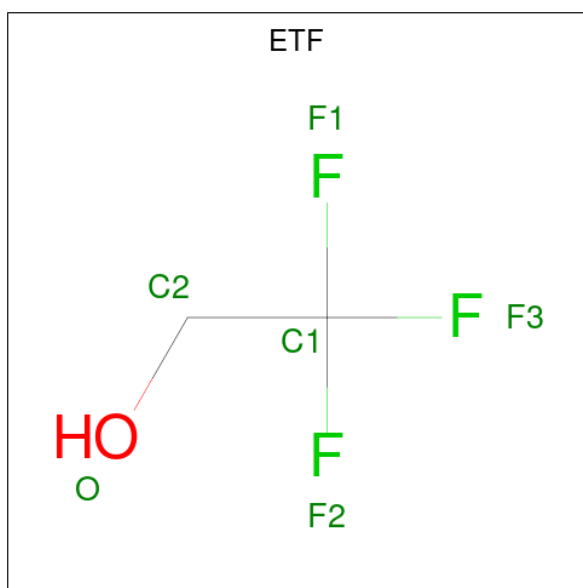
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is S-1,2-PROPANEDIOL (CCD ID: PGO) (formula:  $C_3H_8O_2$ ).



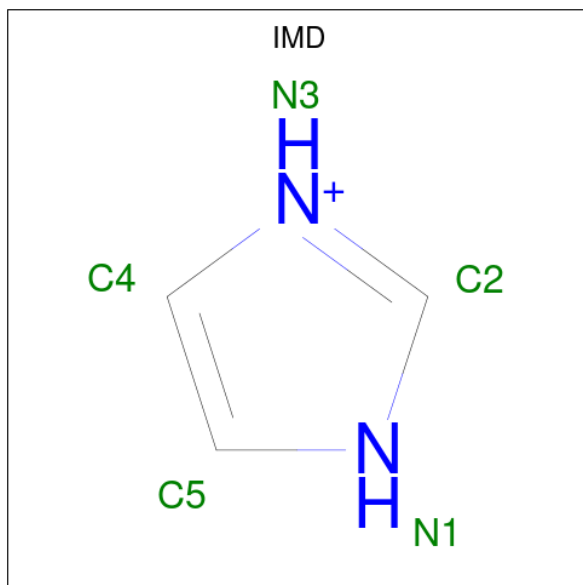
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			5	3	2		
5	A	1	Total	C	O	0	0
			5	3	2		
5	A	1	Total	C	O	0	0
			5	3	2		

- Molecule 6 is TRIFLUOROETHANOL (CCD ID: ETF) (formula:  $C_2H_3F_3O$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	F	O		
6	A	1	6	2	3	1	0	0

- Molecule 7 is IMIDAZOLE (CCD ID: IMD) (formula:  $C_3H_5N_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
7	A	1	5	3	2	0	0
7	A	1	5	3	2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	N	0	0
			5	3	2		
7	A	1	Total	C	N	0	0
			5	3	2		
7	A	1	Total	C	N	0	0
			5	3	2		

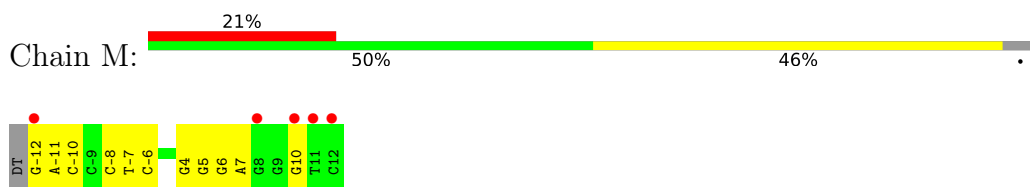
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	3	Total	O	0	0
			3	3		
8	A	52	Total	O	0	0
			52	52		

### 3 Residue-property plots [i](#)

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: BMR promoter DNA



- Molecule 2: Multidrug-efflux transporter 1 regulator



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.48Å 105.48Å 147.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.17 – 2.80 47.17 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.17-2.80) 98.8 (47.17-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.26 (at 2.81Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.225 , 0.248 0.219 , 0.245	Depositor DCC
$R_{free}$ test set	1072 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.6	Xtrriage
Anisotropy	0.411	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2868	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ETF, FLC, PGO, IMD

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	M	0.32	0/524	0.65	0/807
2	A	0.49	0/2334	0.92	8/3152 (0.3%)
All	All	0.46	0/2858	0.87	8/3959 (0.2%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	212	ILE	N-CA-C	-10.18	97.47	107.55
2	A	259	HIS	N-CA-C	6.55	122.09	114.62
2	A	190	ILE	N-CA-C	-5.98	99.87	108.48
2	A	37	ASP	CA-C-N	5.49	125.16	119.56
2	A	37	ASP	C-N-CA	5.49	125.16	119.56

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	M	468	0	259	10	0
2	A	2285	0	2285	72	0
3	A	1	0	0	0	1
4	A	13	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	15	0	24	1	0
6	A	6	0	3	0	0
7	A	25	0	25	0	0
8	A	52	0	0	2	0
8	M	3	0	0	1	0
All	All	2868	0	2601	81	1

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 15.

The worst 5 of 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:M:-11:DA:H2''	1:M:-10:DC:H5'	1.49	0.91
2:A:156:LYS:HG2	2:A:167:ASN:HD21	1.41	0.84
2:A:243:ARG:HB2	2:A:245:LEU:HG	1.64	0.77
2:A:156:LYS:HG2	2:A:167:ASN:ND2	2.02	0.75
2:A:264:LYS:HD3	2:A:265:GLN:N	2.01	0.74

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
3:A:501:ZN:ZN	3:A:501:ZN:ZN[8_665]	1.11	1.09

## 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
2	A	275/284 (97%)	253 (92%)	20 (7%)	2 (1%)	18 47

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	119	PRO
2	A	202	SER

### 5.3.2 Protein sidechains [i](#)

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
2	A	253/262 (97%)	236 (93%)	17 (7%)	15 42

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	219	CYS
2	A	269	ARG
2	A	138	GLU
2	A	140	GLU
2	A	146	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	115	GLN
2	A	136	GLN
2	A	167	ASN
2	A	146	ASN
2	A	90	GLN

### 5.3.3 RNA [i](#)

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 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	IMD	A	305	-	5,5,5	0.92	0	5,5,5	0.56	0
7	IMD	A	303	-	5,5,5	0.87	0	5,5,5	0.55	0
5	PGO	A	600	-	4,4,4	0.50	0	4,4,4	1.36	1 (25%)
6	ETF	A	901	-	5,5,5	0.32	0	7,7,7	0.78	0
5	PGO	A	602	-	4,4,4	0.41	0	4,4,4	1.40	1 (25%)
7	IMD	A	306	-	5,5,5	0.87	0	5,5,5	0.53	0
7	IMD	A	302	-	5,5,5	1.01	0	5,5,5	0.51	0
5	PGO	A	604	-	4,4,4	0.45	0	4,4,4	1.34	1 (25%)
7	IMD	A	304	-	5,5,5	0.85	0	5,5,5	0.59	0
4	FLC	A	756	-	12,12,12	4.50	3 (25%)	17,17,17	2.26	8 (47%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	IMD	A	305	-	-	-	0/1/1/1
7	IMD	A	303	-	-	-	0/1/1/1
5	PGO	A	600	-	-	2/2/2/2	-
6	ETF	A	901	-	-	0/3/3/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGO	A	602	-	-	2/2/2/2	-
7	IMD	A	306	-	-	-	0/1/1/1
7	IMD	A	302	-	-	-	0/1/1/1
5	PGO	A	604	-	-	2/2/2/2	-
7	IMD	A	304	-	-	-	0/1/1/1
4	FLC	A	756	-	-	3/16/16/16	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	756	FLC	CB-CBC	13.11	1.67	1.53
4	A	756	FLC	CG-CB	7.42	1.63	1.54
4	A	756	FLC	OB1-CBC	2.17	1.28	1.22

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	756	FLC	CB-CA-CAC	4.58	126.44	113.92
4	A	756	FLC	CB-CG-CGC	4.00	124.85	113.92
4	A	756	FLC	OB2-CBC-CB	3.50	119.86	113.14
4	A	756	FLC	OA1-CAC-CA	-2.77	115.11	122.95
5	A	602	PGO	C3-C2-C1	2.63	121.62	110.80

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	756	FLC	CA-CB-CG-CGC
4	A	756	FLC	CBC-CB-CG-CGC
5	A	600	PGO	O1-C1-C2-C3
5	A	600	PGO	O1-C1-C2-O2
5	A	602	PGO	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	602	PGO	1	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	M	23/24 (95%)	1.40	5 (21%) <b>2</b> <b>2</b>	44, 82, 111, 126	1 (4%)
2	A	277/284 (97%)	0.18	12 (4%) 40 31	38, 56, 91, 107	0
All	All	300/308 (97%)	0.27	17 (5%) 29 22	38, 59, 95, 126	1 (0%)

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	12	DC	13.0
2	A	278	ASP	10.6
2	A	118	TYR	4.0
2	A	277	LEU	3.8
2	A	201	SER	3.2

### 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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
5	PGO	A	600	5/5	0.74	0.39	85,86,88,88	0
7	IMD	A	305	5/5	0.83	0.41	106,106,106,107	0
4	FLC	A	756	13/13	0.84	0.24	92,97,110,111	0
6	ETF	A	901	6/6	0.90	0.24	126,127,128,128	0
7	IMD	A	304	5/5	0.93	0.21	83,85,86,86	0
5	PGO	A	604	5/5	0.93	0.19	79,79,79,80	0
7	IMD	A	306	5/5	0.93	0.26	94,94,94,94	0
7	IMD	A	302	5/5	0.95	0.15	68,69,70,72	0
7	IMD	A	303	5/5	0.96	0.16	83,83,85,85	0
5	PGO	A	602	5/5	0.98	0.09	49,50,52,53	0
3	ZN	A	501	1/1	0.99	0.02	79,79,79,79	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.