



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:07 PM GMT

PDB ID : 4BEJ  
Title : Nucleotide-free Dynamin 1-like protein (DNM1L, DRP1, DLP1)  
Authors : Froehlich, C.; Schwefel, D.; Faelber, K.; Daumke, O.  
Deposited on : 2013-03-11  
Resolution : 3.48 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  
<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  
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

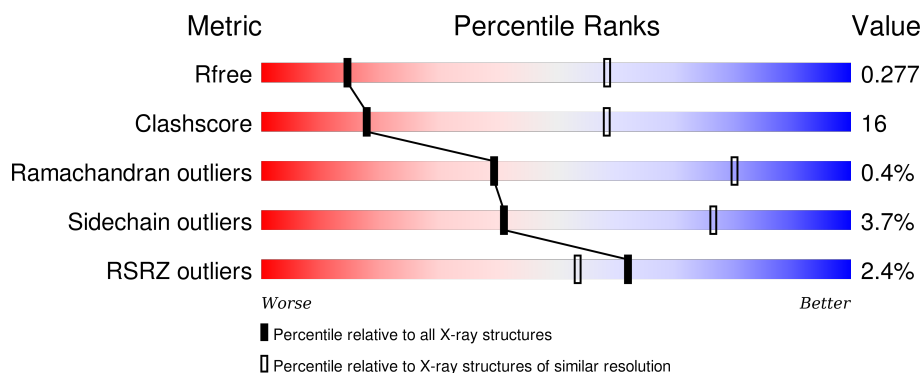
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.48 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	1173 (3.60-3.36)
Clashscore	102246	1010 (3.58-3.38)
Ramachandran outliers	100387	1245 (3.60-3.36)
Sidechain outliers	100360	1246 (3.60-3.36)
RSRZ outliers	91569	1180 (3.60-3.36)

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	617	<div> <div> <div></div> <div>58%</div> <div>29%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	617	<div> <div> <div>3%</div> <div>55%</div> <div>32%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	617	<div> <div> <div>2%</div> <div>53%</div> <div>31%</div> <div>••</div> <div>13%</div> </div> </div>
1	D	617	<div> <div> <div>2%</div> <div>57%</div> <div>28%</div> <div>•</div> <div>12%</div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 17076 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 DYNAMIN 1-LIKE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	540	Total	C	N	O	S	0	0	0
			4263	2701	740	801	21			
1	B	547	Total	C	N	O	S	0	0	0
			4313	2728	755	810	20			
1	C	534	Total	C	N	O	S	0	0	0
			4218	2678	736	785	19			
1	D	540	Total	C	N	O	S	0	0	0
			4282	2717	748	797	20			

There are 44 discrepancies between the modelled and reference sequences:

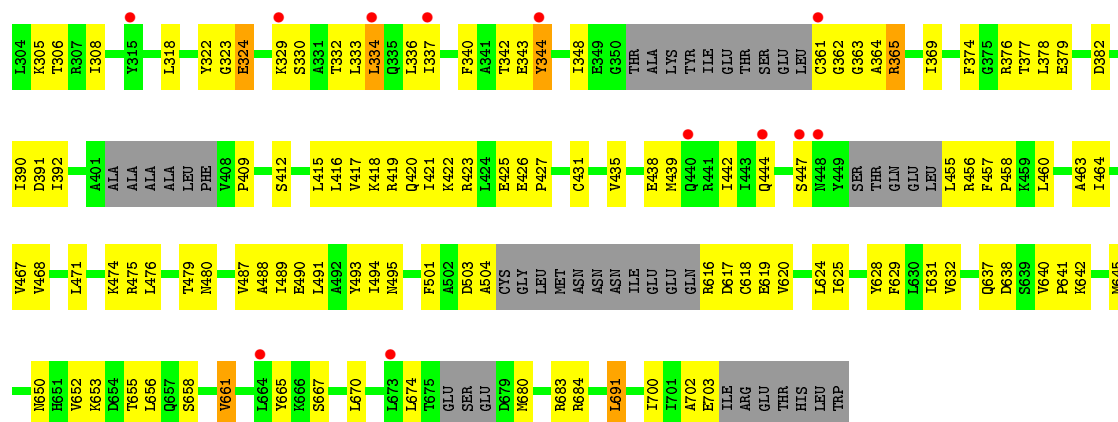
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	EXPRESSION TAG	UNP O00429
A	-5	PRO	-	EXPRESSION TAG	UNP O00429
A	-4	HIS	-	EXPRESSION TAG	UNP O00429
A	-3	MET	-	EXPRESSION TAG	UNP O00429
A	-2	GLY	-	EXPRESSION TAG	UNP O00429
A	-1	GLY	-	EXPRESSION TAG	UNP O00429
A	0	SER	-	EXPRESSION TAG	UNP O00429
A	401	ALA	GLY	ENGINEERED MUTATION	UNP O00429
A	402	ALA	PRO	ENGINEERED MUTATION	UNP O00429
A	403	ALA	ARG	ENGINEERED MUTATION	UNP O00429
A	404	ALA	PRO	ENGINEERED MUTATION	UNP O00429
B	-6	GLY	-	EXPRESSION TAG	UNP O00429
B	-5	PRO	-	EXPRESSION TAG	UNP O00429
B	-4	HIS	-	EXPRESSION TAG	UNP O00429
B	-3	MET	-	EXPRESSION TAG	UNP O00429
B	-2	GLY	-	EXPRESSION TAG	UNP O00429
B	-1	GLY	-	EXPRESSION TAG	UNP O00429
B	0	SER	-	EXPRESSION TAG	UNP O00429
B	401	ALA	GLY	ENGINEERED MUTATION	UNP O00429
B	402	ALA	PRO	ENGINEERED MUTATION	UNP O00429
B	403	ALA	ARG	ENGINEERED MUTATION	UNP O00429

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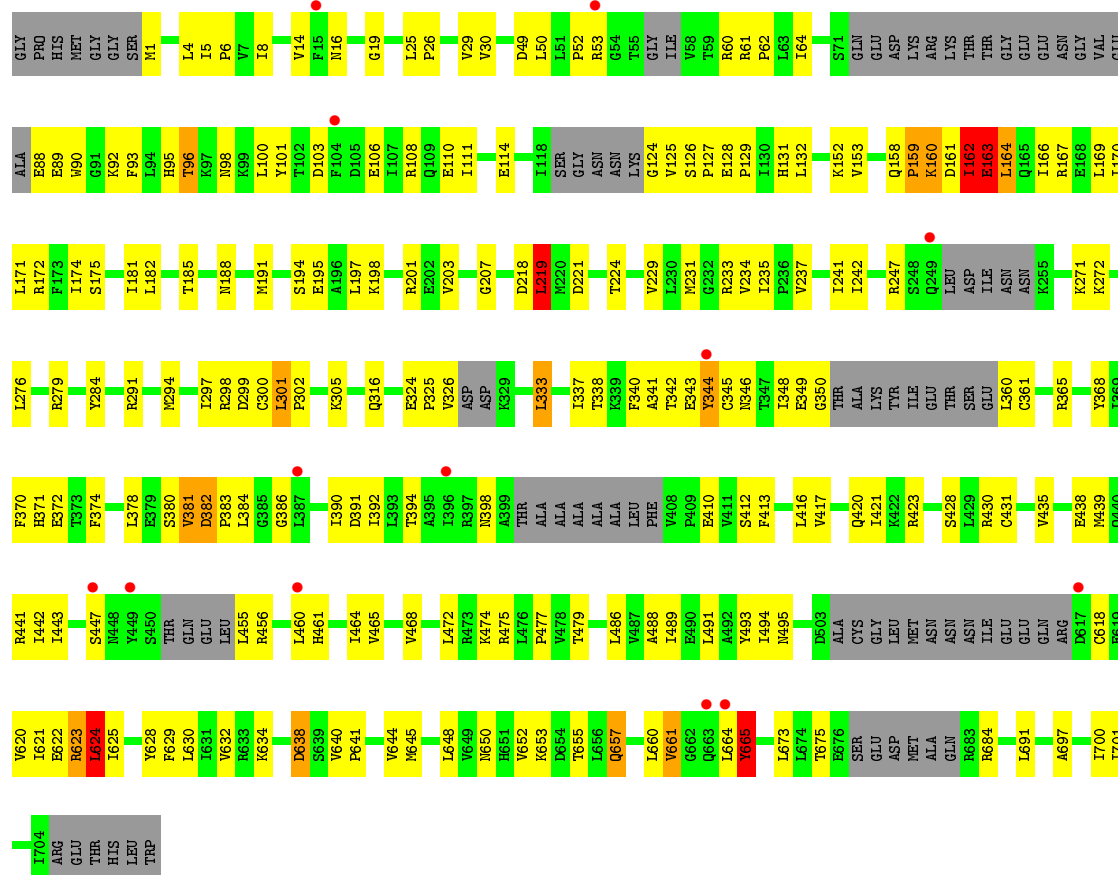
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Chain	Residue	Modelled	Actual	Comment	Reference
B	404	ALA	PRO	ENGINEERED MUTATION	UNP O00429
C	-6	GLY	-	EXPRESSION TAG	UNP O00429
C	-5	PRO	-	EXPRESSION TAG	UNP O00429
C	-4	HIS	-	EXPRESSION TAG	UNP O00429
C	-3	MET	-	EXPRESSION TAG	UNP O00429
C	-2	GLY	-	EXPRESSION TAG	UNP O00429
C	-1	GLY	-	EXPRESSION TAG	UNP O00429
C	0	SER	-	EXPRESSION TAG	UNP O00429
C	401	ALA	GLY	ENGINEERED MUTATION	UNP O00429
C	402	ALA	PRO	ENGINEERED MUTATION	UNP O00429
C	403	ALA	ARG	ENGINEERED MUTATION	UNP O00429
C	404	ALA	PRO	ENGINEERED MUTATION	UNP O00429
D	-6	GLY	-	EXPRESSION TAG	UNP O00429
D	-5	PRO	-	EXPRESSION TAG	UNP O00429
D	-4	HIS	-	EXPRESSION TAG	UNP O00429
D	-3	MET	-	EXPRESSION TAG	UNP O00429
D	-2	GLY	-	EXPRESSION TAG	UNP O00429
D	-1	GLY	-	EXPRESSION TAG	UNP O00429
D	0	SER	-	EXPRESSION TAG	UNP O00429
D	401	ALA	GLY	ENGINEERED MUTATION	UNP O00429
D	402	ALA	PRO	ENGINEERED MUTATION	UNP O00429
D	403	ALA	ARG	ENGINEERED MUTATION	UNP O00429
D	404	ALA	PRO	ENGINEERED MUTATION	UNP O00429

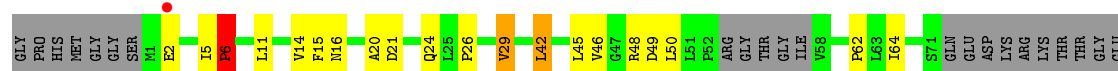


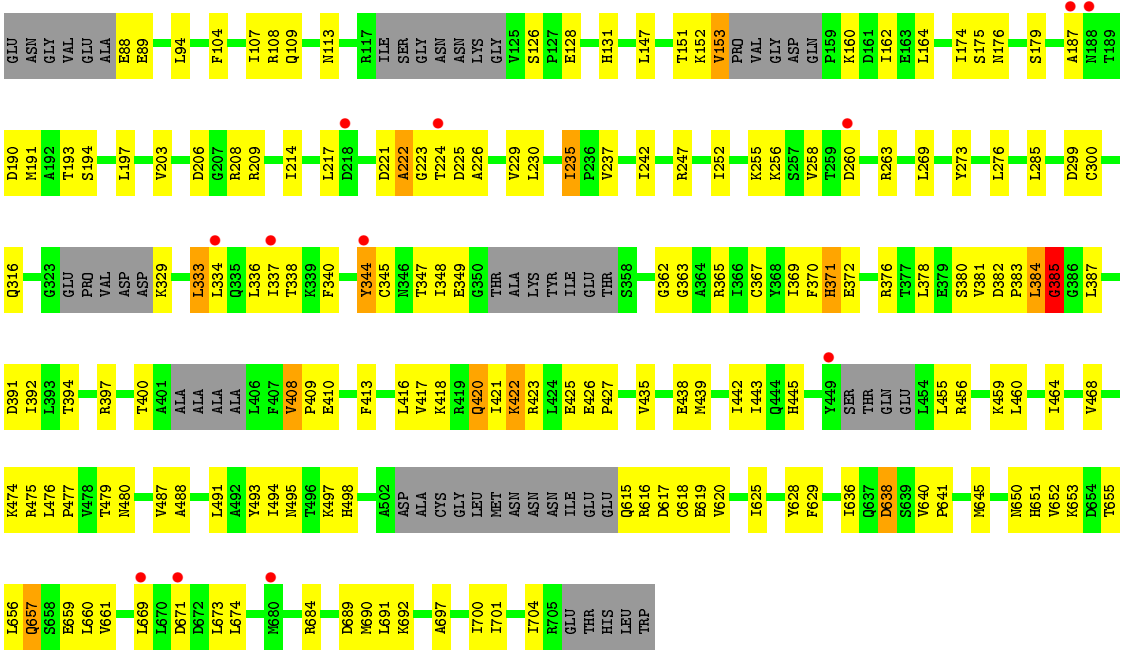


### • Molecule 1: DYNAMIN 1-LIKE PROTEIN



### • Molecule 1: DYNAMIN 1-LIKE PROTEIN





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.47Å 80.77Å 208.27Å 90.00° 93.45° 90.00°	Depositor
Resolution (Å)	47.57 – 3.48 48.54 – 3.48	Depositor EDS
% Data completeness (in resolution range)	97.3 (47.57-3.48) 97.3 (48.54-3.48)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 3.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.251 , 0.276 0.251 , 0.277	Depositor DCC
$R_{free}$ test set	2119 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	74.8	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 31.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 42403 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	17076	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% 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

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	0.31	0/4314	0.72	1/5830 (0.0%)
1	B	0.32	0/4366	0.76	7/5900 (0.1%)
1	C	0.39	3/4271 (0.1%)	0.81	16/5771 (0.3%)
1	D	0.34	1/4335 (0.0%)	0.77	8/5855 (0.1%)
All	All	0.34	4/17286 (0.0%)	0.76	32/23356 (0.1%)

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	B	0	1
1	C	0	2
1	D	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	LYS	CD-CE	7.11	1.69	1.51
1	C	160	LYS	CB-CG	7.11	1.71	1.52
1	D	6	PRO	CG-CD	6.52	1.72	1.50
1	C	160	LYS	CA-CB	5.12	1.65	1.53

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	164	LEU	CA-CB-CG	-9.36	93.78	115.30
1	D	387	LEU	CA-CB-CG	9.26	136.61	115.30
1	D	6	PRO	CA-N-CD	-8.55	99.52	111.50
1	B	334	LEU	CA-CB-CG	-8.02	96.86	115.30
1	D	385	GLY	C-N-CA	7.45	137.95	122.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	250	LEU	Peptide
1	C	361	CYS	Peptide
1	C	381	VAL	Peptide
1	D	385	GLY	Peptide

## 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	4263	0	4407	139	0
1	B	4313	0	4462	145	0
1	C	4218	0	4382	157	0
1	D	4282	0	4448	127	0
All	All	17076	0	17699	548	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 16.

The worst 5 of 548 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:616:ARG:HB2	1:A:619:GLU:HB2	1.43	0.99
1:B:249:GLN:HA	1:B:252:ILE:HB	1.53	0.90
1:A:214:ILE:HG13	1:A:241:ILE:HD11	1.54	0.89
1:B:175:SER:HA	1:B:203:VAL:HG11	1.62	0.81
1:A:113:ASN:ND2	1:C:231:MET:O	2.13	0.80

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	518/617 (84%)	487 (94%)	28 (5%)	3 (1%)	30	74
1	B	529/617 (86%)	497 (94%)	31 (6%)	1 (0%)	52	87
1	C	512/617 (83%)	479 (94%)	30 (6%)	3 (1%)	30	74
1	D	520/617 (84%)	498 (96%)	20 (4%)	2 (0%)	39	80
All	All	2079/2468 (84%)	1961 (94%)	109 (5%)	9 (0%)	39	80

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	222	ALA
1	A	323	GLY
1	B	665	TYR
1	A	387	LEU
1	C	19	GLY

### 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	484/546 (89%)	471 (97%)	13 (3%)	52	82
1	B	488/546 (89%)	467 (96%)	21 (4%)	35	74
1	C	480/546 (88%)	461 (96%)	19 (4%)	38	75
1	D	487/546 (89%)	468 (96%)	19 (4%)	39	76
All	All	1939/2184 (89%)	1867 (96%)	72 (4%)	41	76

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	674	LEU
1	C	326	VAL
1	D	410	GLU
1	B	691	LEU
1	C	96	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	95	HIS
1	C	113	ASN
1	D	16	ASN
1	B	651	HIS
1	C	131	HIS

### 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 ⓘ

There are no ligands in this entry.

## 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 [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	A	540/617 (87%)	0.09	7 (1%) 79 71	4, 48, 90, 140	0
1	B	547/617 (88%)	0.23	18 (3%) 50 42	8, 58, 105, 141	0
1	C	534/617 (86%)	0.12	13 (2%) 62 53	8, 59, 104, 128	0
1	D	540/617 (87%)	0.14	13 (2%) 62 53	9, 54, 97, 126	0
All	All	2161/2468 (87%)	0.15	51 (2%) 62 53	4, 54, 102, 141	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	679	ASP	4.4
1	C	617	ASP	4.4
1	C	249	GLN	4.3
1	D	671	ASP	4.2
1	B	151	THR	3.6

### 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.