



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2018 – 08:46 PM EST

PDB ID : 6B72  
Title : A novel HIV-1 Nef dimer interface induced by a single octyl-glucoside molecule  
Authors : Wu, M.; Augelli-Szafran, C.E.; Ptak, R.G.; Smithgall, T.E.  
Deposited on : 2017-10-03  
Resolution : 3.20 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  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
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) : rb-20030736

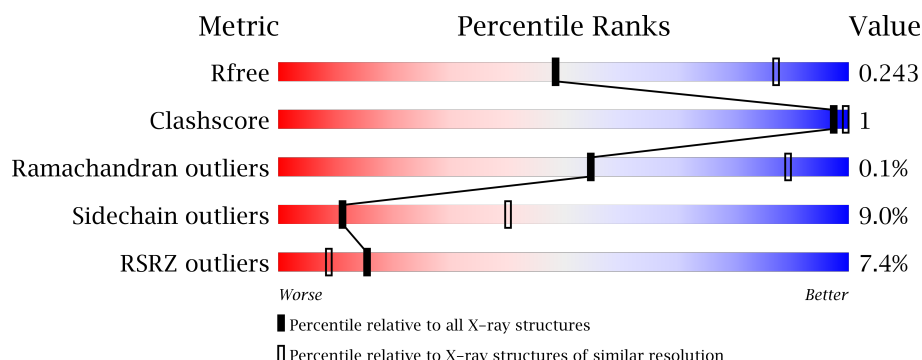
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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	151	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>9%</div> <div>18%</div> </div> </div>
1	B	151	<div> <div>7%</div> <div> <div></div> <div>72%</div> <div>7%</div> <div>20%</div> </div> </div>
1	C	151	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>7%</div> <div>19%</div> </div> </div>
1	D	151	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>7%</div> <div>19%</div> </div> </div>
1	E	151	<div> <div>9%</div> <div> <div></div> <div>70%</div> <div>9%</div> <div>21%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	151	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BOG	C	301	-	-	-	X
2	BOG	F	301	-	-	-	X

## 2 Entry composition [i](#)

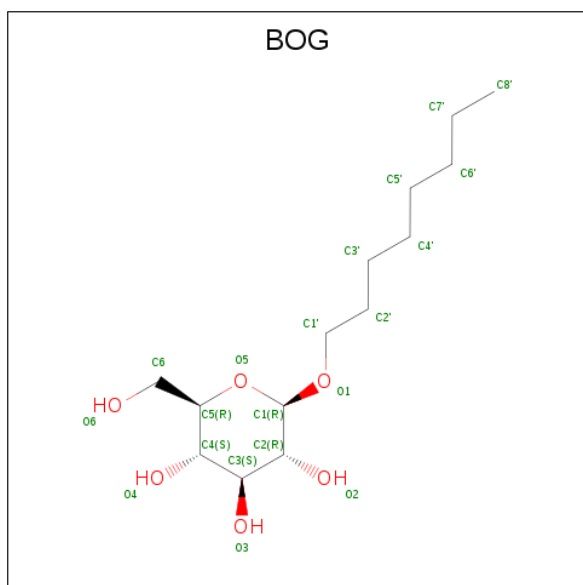
There are 2 unique types of molecules in this entry. The entry contains 6243 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Protein Nef.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	124	Total	C	N	O	S	0	0	0
			1049	690	174	181	4			
1	B	121	Total	C	N	O	S	0	0	0
			1027	678	171	174	4			
1	C	122	Total	C	N	O	S	0	0	0
			1036	683	172	177	4			
1	D	122	Total	C	N	O	S	0	0	0
			1036	683	172	177	4			
1	E	119	Total	C	N	O	S	0	0	0
			1009	667	168	170	4			
1	F	121	Total	C	N	O	S	0	0	0
			1026	677	171	174	4			

- Molecule 2 is B-OCTYLGLUCOSIDE (three-letter code: BOG) (formula:  $C_{14}H_{28}O_6$ ).

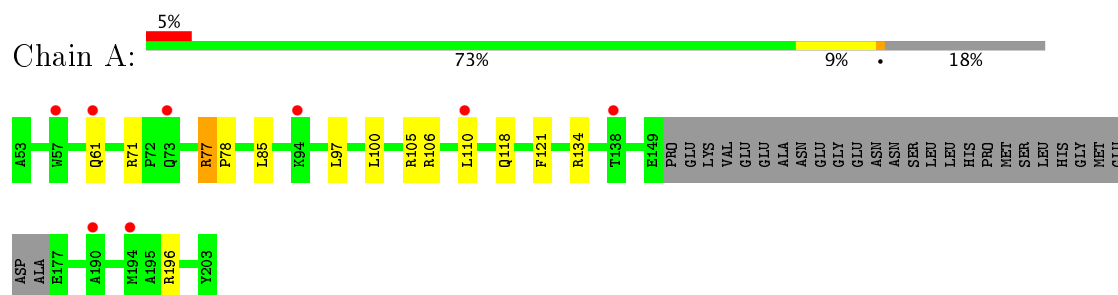


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 20	C 14	O 6	0	0
2	C	1	Total 20	C 14	O 6	0	0
2	F	1	Total 20	C 14	O 6	0	0

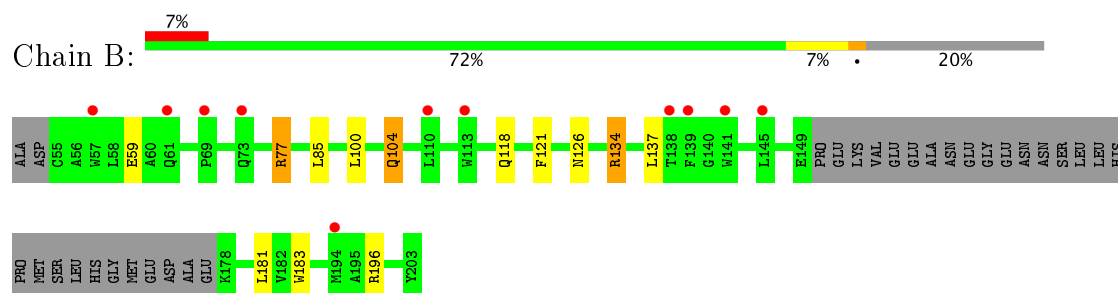
### 3 Residue-property plots [i](#)

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.

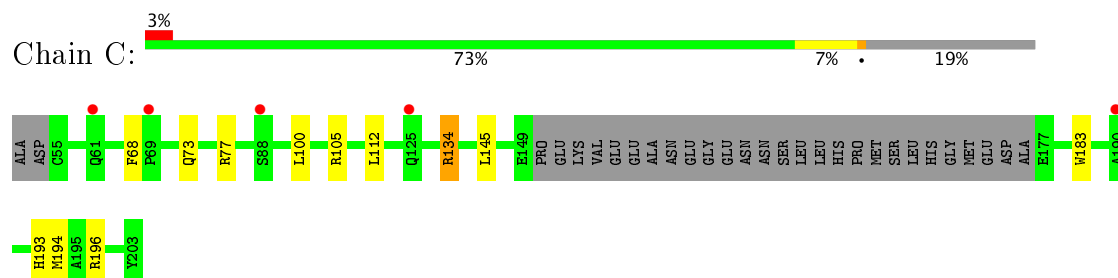
#### • Molecule 1: Protein Nef



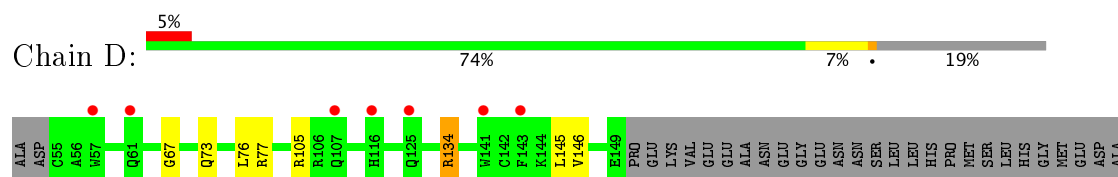
#### • Molecule 1: Protein Nef



#### • Molecule 1: Protein Nef

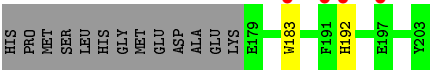
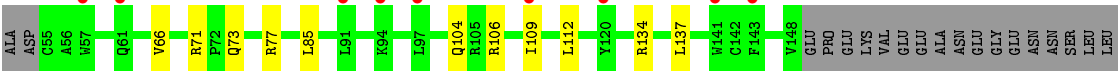


#### • Molecule 1: Protein Nef

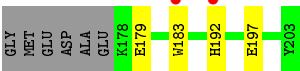
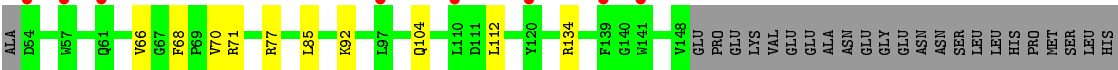




• Molecule 1: Protein Nef



• Molecule 1: Protein Nef



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.58Å 109.58Å 247.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	94.90 – 3.20 88.59 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (94.90-3.20) 100.0 (88.59-3.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.00 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.233 , 0.251 0.233 , 0.243	Depositor DCC
$R_{free}$ test set	1494 reflections (5.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	109.6	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 85.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6243	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.74 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.6149e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: BOG

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	0.39	0/1088	0.60	0/1480
1	B	0.39	0/1066	0.59	0/1450
1	C	0.38	0/1075	0.60	0/1462
1	D	0.39	0/1075	0.59	0/1462
1	E	0.40	0/1048	0.60	0/1427
1	F	0.38	0/1065	0.64	0/1449
All	All	0.39	0/6417	0.60	0/8730

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	D	0	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	67	GLY	Peptide
1	F	66	VAL	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	1049	0	1001	3	0
1	B	1027	0	986	3	0
1	C	1036	0	992	3	0
1	D	1036	0	992	2	0
1	E	1009	0	967	2	0
1	F	1026	0	984	0	0
2	A	20	0	28	0	0
2	C	20	0	28	0	0
2	F	20	0	28	0	0
All	All	6243	0	6006	12	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 1.

All (12) 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:B:77:ARG:NH1	1:B:118:GLN:O	2.36	0.59
1:A:97:LEU:HD21	1:A:110:LEU:HD22	1.90	0.53
1:D:134:ARG:HB2	1:D:145:LEU:HB2	1.91	0.52
1:B:134:ARG:NH2	1:B:181:LEU:HD21	2.27	0.48
1:D:193:HIS:ND1	1:D:196:ARG:HB2	2.30	0.46
1:B:104:GLN:HE21	1:B:104:GLN:HA	1.83	0.43
1:A:77:ARG:NH1	1:A:118:GLN:O	2.49	0.43
1:C:193:HIS:ND1	1:C:196:ARG:HB2	2.33	0.43
1:C:134:ARG:HB2	1:C:145:LEU:HB2	2.01	0.42
1:A:100:LEU:HD22	1:A:106:ARG:NH1	2.36	0.41
1:C:112:LEU:CD1	1:E:109:ILE:HD12	2.51	0.41
1:E:66:VAL:O	1:E:66:VAL:HG23	2.22	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	120/151 (80%)	109 (91%)	10 (8%)	1 (1%)	22	65
1	B	117/151 (78%)	110 (94%)	7 (6%)	0	100	100
1	C	118/151 (78%)	112 (95%)	6 (5%)	0	100	100
1	D	118/151 (78%)	113 (96%)	5 (4%)	0	100	100
1	E	115/151 (76%)	105 (91%)	10 (9%)	0	100	100
1	F	117/151 (78%)	109 (93%)	8 (7%)	0	100	100
All	All	705/906 (78%)	658 (93%)	46 (6%)	1 (0%)	55	89

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	PRO

### 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	109/132 (83%)	101 (93%)	8 (7%)	16	53
1	B	107/132 (81%)	96 (90%)	11 (10%)	8	33
1	C	108/132 (82%)	100 (93%)	8 (7%)	16	52
1	D	108/132 (82%)	101 (94%)	7 (6%)	20	58
1	E	105/132 (80%)	94 (90%)	11 (10%)	8	32
1	F	107/132 (81%)	94 (88%)	13 (12%)	6	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	644/792 (81%)	586 (91%)	58 (9%)	11	40

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	71	ARG
1	A	77	ARG
1	A	85	LEU
1	A	105	ARG
1	A	121	PHE
1	A	134	ARG
1	A	196	ARG
1	B	59	GLU
1	B	77	ARG
1	B	85	LEU
1	B	100	LEU
1	B	104	GLN
1	B	121	PHE
1	B	126	ASN
1	B	134	ARG
1	B	137	LEU
1	B	183	TRP
1	B	196	ARG
1	C	68	PHE
1	C	73	GLN
1	C	77	ARG
1	C	100	LEU
1	C	105	ARG
1	C	134	ARG
1	C	183	TRP
1	C	194	MET
1	D	73	GLN
1	D	76	LEU
1	D	77	ARG
1	D	105	ARG
1	D	134	ARG
1	D	146	VAL
1	D	183	TRP
1	E	71	ARG
1	E	73	GLN
1	E	77	ARG

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Mol	Chain	Res	Type
1	E	85	LEU
1	E	104	GLN
1	E	106	ARG
1	E	112	LEU
1	E	134	ARG
1	E	137	LEU
1	E	183	TRP
1	E	192	HIS
1	F	68	PHE
1	F	70	VAL
1	F	71	ARG
1	F	77	ARG
1	F	85	LEU
1	F	92	LYS
1	F	104	GLN
1	F	112	LEU
1	F	134	ARG
1	F	179	GLU
1	F	183	TRP
1	F	192	HIS
1	F	197	GLU

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	61	GLN
1	B	104	GLN
1	C	61	GLN
1	C	73	GLN
1	D	73	GLN
1	E	73	GLN
1	E	104	GLN
1	F	61	GLN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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	$\# Z  > 2$
2	BOG	A	601	-	20,20,20	0.59	1 (5%)	25,25,25	0.47	0
2	BOG	C	301	-	20,20,20	0.53	0	25,25,25	0.60	0
2	BOG	F	301	-	20,20,20	0.54	0	25,25,25	0.59	0

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
2	BOG	A	601	-	-	0/11/31/31	0/1/1/1
2	BOG	C	301	-	-	0/11/31/31	0/1/1/1
2	BOG	F	301	-	-	0/11/31/31	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	BOG	O1-C1	2.03	1.43	1.40

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	124/151 (82%)	0.73	8 (6%)	20 11	91, 114, 159, 177	0
1	B	121/151 (80%)	0.81	11 (9%)	10 6	92, 110, 150, 186	0
1	C	122/151 (80%)	0.76	5 (4%)	38 25	97, 115, 181, 208	0
1	D	122/151 (80%)	0.75	7 (5%)	24 14	91, 111, 153, 197	0
1	E	119/151 (78%)	0.80	13 (10%)	6 4	98, 119, 161, 195	0
1	F	121/151 (80%)	0.81	10 (8%)	12 7	96, 119, 162, 197	0
All	All	729/906 (80%)	0.78	54 (7%)	15 9	91, 115, 167, 208	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	192	HIS	5.1
1	A	57	TRP	4.9
1	F	61	GLN	4.6
1	D	57	TRP	4.4
1	B	57	TRP	4.3
1	C	61	GLN	4.2
1	B	61	GLN	3.9
1	E	192	HIS	3.9
1	F	54	ASP	3.8
1	B	73	GLN	3.5
1	E	61	GLN	3.5
1	E	57	TRP	3.2
1	E	183	TRP	3.1
1	F	57	TRP	2.9
1	D	61	GLN	2.9
1	F	141	TRP	2.9
1	A	73	GLN	2.9
1	E	120	TYR	2.9
1	B	194	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	94	LYS	2.7
1	D	107	GLN	2.7
1	C	69	PRO	2.7
1	E	143	PHE	2.7
1	E	141	TRP	2.7
1	F	110	LEU	2.6
1	A	194	MET	2.6
1	E	97	LEU	2.6
1	A	110	LEU	2.5
1	B	141	TRP	2.5
1	B	110	LEU	2.5
1	D	143	PHE	2.5
1	F	139	PHE	2.4
1	A	94	LYS	2.4
1	F	97	LEU	2.4
1	F	183	TRP	2.4
1	D	141	TRP	2.3
1	A	61	GLN	2.3
1	B	69	PRO	2.3
1	E	197	GLU	2.2
1	E	109	ILE	2.2
1	E	191	PHE	2.2
1	D	116	HIS	2.2
1	A	138	THR	2.2
1	F	120	TYR	2.2
1	B	138	THR	2.2
1	C	190	ALA	2.1
1	B	145	LEU	2.1
1	C	88	SER	2.1
1	B	139	PHE	2.1
1	B	113	TRP	2.1
1	D	125	GLN	2.1
1	A	190	ALA	2.0
1	C	125	GLN	2.0
1	E	91	LEU	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 [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	BOG	F	301	20/20	0.85	0.58	3.29	115,126,131,133	0
2	BOG	C	301	20/20	0.85	0.53	2.47	124,127,133,133	0
2	BOG	A	601	20/20	0.81	0.36	-0.39	89,109,121,125	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.