



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 03:10 AM GMT

PDB ID : 4CDG  
Title : Crystal structure of the Bloom's syndrome helicase BLM in complex with Nanobody  
Authors : Newman, J.A.; Savitsky, P.; Allerston, C.K.; Pike, A.C.W.; Pardon, E.; Steyaert, J.; Arrowsmith, C.H.; Von Delft, F.; Bountra, C.; Edwards, A.; Gileadi, O.  
Deposited on : 2013-10-31  
Resolution : 2.79 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>

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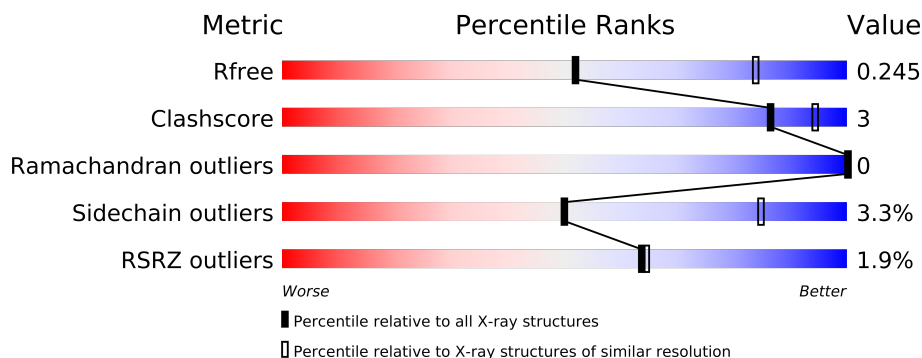
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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 2.79 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	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (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 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	673	
1	B	673	
2	C	147	
2	D	147	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	ZN	A	1643	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11711 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 BLOOM SYNDROME PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	625	Total	C	N	O	S	0	0	0
			4910	3127	834	916	33			
1	B	616	Total	C	N	O	S	0	0	0
			4858	3091	823	910	34			

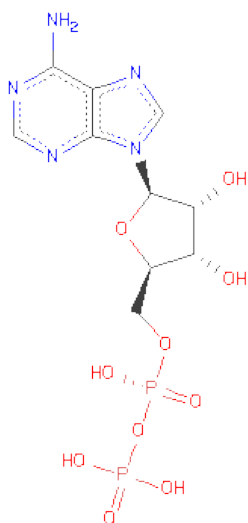
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	634	SER	-	EXPRESSION TAG	UNP P54132
A	635	MET	-	EXPRESSION TAG	UNP P54132
A	1299	MET	-	EXPRESSION TAG	UNP P54132
A	1300	SER	-	EXPRESSION TAG	UNP P54132
A	1301	GLU	-	EXPRESSION TAG	UNP P54132
A	1302	ASN	-	EXPRESSION TAG	UNP P54132
A	1303	LEU	-	EXPRESSION TAG	UNP P54132
A	1304	TYR	-	EXPRESSION TAG	UNP P54132
A	1305	PHE	-	EXPRESSION TAG	UNP P54132
A	1306	GLN	-	EXPRESSION TAG	UNP P54132
B	634	SER	-	EXPRESSION TAG	UNP P54132
B	635	MET	-	EXPRESSION TAG	UNP P54132
B	1299	MET	-	EXPRESSION TAG	UNP P54132
B	1300	SER	-	EXPRESSION TAG	UNP P54132
B	1301	GLU	-	EXPRESSION TAG	UNP P54132
B	1302	ASN	-	EXPRESSION TAG	UNP P54132
B	1303	LEU	-	EXPRESSION TAG	UNP P54132
B	1304	TYR	-	EXPRESSION TAG	UNP P54132
B	1305	PHE	-	EXPRESSION TAG	UNP P54132
B	1306	GLN	-	EXPRESSION TAG	UNP P54132

- Molecule 2 is a protein called NANOBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	122	Total	C	N	O	S	0	0	0
			942	587	168	181	6			
2	D	122	Total	C	N	O	S	0	0	0
			945	589	168	182	6			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

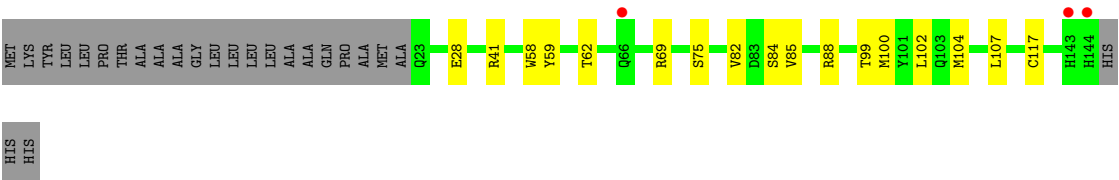
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula:  $Zn$ ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		



● Molecule 2: NANOBODY

Chain D: 



HIS  
HIS

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.67Å 88.42Å 95.12Å 69.39° 89.84° 77.07°	Depositor
Resolution (Å)	42.88 – 2.79 57.95 – 2.79	Depositor EDS
% Data completeness (in resolution range)	98.5 (42.88-2.79) 98.6 (57.95-2.79)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.93 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.206 , 0.245 0.209 , 0.245	Depositor DCC
$R_{free}$ test set	2170 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.5	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 39.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 43190 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11711	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.07% 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: ZN, ADP

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	0.21	0/5007	0.39	0/6771
1	B	0.22	0/4953	0.39	0/6692
2	C	0.22	0/962	0.37	0/1304
2	D	0.22	0/964	0.38	0/1305
All	All	0.22	0/11886	0.38	0/16072

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	4910	0	4821	24	0
1	B	4858	0	4761	23	0
2	C	942	0	891	6	0
2	D	945	0	903	7	0
3	A	27	0	12	0	0
3	B	27	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11711	0	11400	59	0

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 3.

All (59) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:676:ILE:HD13	1:B:701:LEU:HD23	1.69	0.74
1:A:1211:ARG:NH2	1:A:1251:GLU:O	2.27	0.67
1:B:859:ARG:NH1	1:B:978:GLY:O	2.27	0.67
1:A:859:ARG:NH1	1:A:978:GLY:O	2.29	0.66
2:D:59:TYR:OH	2:D:69:ARG:NH1	2.32	0.63
2:D:58:TRP:NE1	2:D:100:MET:SD	2.72	0.63
1:B:1211:ARG:NH2	1:B:1251:GLU:O	2.36	0.58
1:A:643:ARG:NH1	1:B:823:SER:O	2.36	0.58
2:C:59:TYR:OH	2:C:69:ARG:NH1	2.37	0.58
2:C:84:SER:O	2:C:88:ARG:NH1	2.36	0.57
2:C:58:TRP:NE1	2:C:100:MET:SD	2.78	0.56
1:A:1116:ASP:OD1	1:A:1139:ARG:NH2	2.35	0.56
1:A:733:PRO:HB2	1:A:760:ILE:HA	1.89	0.55
1:B:1221:GLU:OE2	1:B:1285:TYR:OH	2.25	0.53
1:B:966:LEU:HD22	1:B:967:PRO:HD2	1.91	0.53
1:B:1046:GLY:O	1:B:1048:ASN:ND2	2.42	0.53
2:D:28:GLU:OE2	2:D:117:CYS:N	2.37	0.52
1:A:671:ASN:ND2	1:A:854:SER:O	2.42	0.52
1:B:1116:ASP:OD1	1:B:1139:ARG:NH2	2.33	0.52
1:A:1221:GLU:OE2	1:A:1285:TYR:OH	2.26	0.52
2:D:84:SER:O	2:D:88:ARG:NH1	2.43	0.51
1:B:1194:ASN:OD1	1:B:1195:SER:N	2.42	0.51
1:A:655:MET:HG3	1:A:701:LEU:HD11	1.93	0.51
1:A:735:THR:HG21	1:A:749:ILE:HD12	1.94	0.50
1:B:671:ASN:ND2	1:B:854:SER:O	2.45	0.50
1:B:662:LYS:NZ	1:B:731:ASP:O	2.45	0.49
2:C:58:TRP:CD1	2:C:102:LEU:HB2	2.49	0.48
2:C:88:ARG:NH2	2:C:111:ASP:OD2	2.46	0.48
1:A:701:LEU:HB3	1:A:702:PRO:HD3	1.96	0.48
2:D:58:TRP:CD1	2:D:102:LEU:HB2	2.49	0.47
1:A:998:VAL:HG12	1:A:1002:LYS:HE3	1.97	0.47
1:A:893:ILE:HD13	1:A:904:MET:HE2	1.97	0.46
1:B:1175:ASN:OD1	1:B:1176:LYS:N	2.49	0.45
1:A:735:THR:OG1	1:A:736:TYR:N	2.48	0.45
1:A:954:ASP:HB2	1:A:979:ARG:NH2	2.32	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:909:GLN:NE2	1:A:915:ALA:O	2.50	0.44
1:B:994:THR:HG22	1:B:996:HIS:H	1.82	0.44
1:B:1064:ASP:OD1	1:B:1065:ASN:N	2.51	0.43
1:B:665:LEU:HD13	3:B:1634:ADP:C6	2.54	0.43
1:B:735:THR:HG22	1:B:760:ILE:HD12	2.00	0.43
1:B:735:THR:OG1	1:B:736:TYR:N	2.51	0.43
1:A:699:TYR:HB3	1:A:827:MET:HE1	2.00	0.43
1:A:1064:ASP:OD1	1:A:1065:ASN:N	2.51	0.43
2:D:104:MET:HE2	2:D:107:LEU:HD21	2.00	0.42
1:A:863:LYS:HG2	1:A:1061:VAL:HA	2.01	0.42
1:B:898:ARG:HG3	1:B:919:HIS:CG	2.54	0.42
1:A:710:THR:HB	1:A:762:LEU:HD13	2.02	0.42
1:B:859:ARG:NH2	1:B:861:ASN:OD1	2.53	0.42
2:D:82:VAL:HG12	2:D:85:VAL:HG22	2.01	0.41
1:B:701:LEU:HB3	1:B:702:PRO:HD3	2.03	0.41
1:A:735:THR:HG22	1:A:760:ILE:HD12	2.02	0.41
1:B:893:ILE:HD13	1:B:904:MET:HE2	2.03	0.41
1:B:1122:LYS:HE3	1:B:1122:LYS:HB3	1.90	0.41
2:C:74:THR:HG23	2:C:76:ALA:H	1.86	0.41
1:A:1277:GLU:N	1:A:1277:GLU:OE1	2.45	0.40
1:A:714:SER:O	1:A:767:PRO:HD3	2.21	0.40
1:A:834:ASN:HA	1:A:835:PRO:HD3	1.91	0.40
1:A:1226:CYS:SG	1:A:1246:LEU:HD21	2.61	0.40
1:B:1277:GLU:N	1:B:1277:GLU:OE1	2.47	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	619/673 (92%)	594 (96%)	25 (4%)	0	100	100
1	B	606/673 (90%)	584 (96%)	22 (4%)	0	100	100
2	C	120/147 (82%)	116 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	120/147 (82%)	116 (97%)	4 (3%)	0	100	100
All	All	1465/1640 (89%)	1410 (96%)	55 (4%)	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	531/601 (88%)	512 (96%)	19 (4%)	47	82
1	B	528/601 (88%)	512 (97%)	16 (3%)	53	87
2	C	99/118 (84%)	96 (97%)	3 (3%)	53	87
2	D	100/118 (85%)	96 (96%)	4 (4%)	42	79
All	All	1258/1438 (88%)	1216 (97%)	42 (3%)	50	85

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	662	LYS
1	A	688	LEU
1	A	709	VAL
1	A	714	SER
1	A	722	ASP
1	A	756	LYS
1	A	789	LEU
1	A	874	VAL
1	A	899	ARG
1	A	910	ARG
1	A	949	PHE
1	A	955	LYS
1	A	994	THR
1	A	1108	ARG
1	A	1121	SER
1	A	1139	ARG
1	A	1156	ASP

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Mol	Chain	Res	Type
1	A	1164	ASN
1	A	1205	VAL
1	B	709	VAL
1	B	714	SER
1	B	722	ASP
1	B	757	ASP
1	B	789	LEU
1	B	816	MET
1	B	899	ARG
1	B	910	ARG
1	B	949	PHE
1	B	955	LYS
1	B	1033	ILE
1	B	1121	SER
1	B	1122	LYS
1	B	1139	ARG
1	B	1156	ASP
1	B	1199	LYS
2	C	41	ARG
2	C	62	THR
2	C	142	HIS
2	D	41	ARG
2	D	62	THR
2	D	75	SER
2	D	99	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	802	GLN
1	A	1021	ASN
1	A	1058	HIS
1	A	1089	GLN
1	B	802	GLN
1	B	975	GLN
1	B	1048	ASN
1	B	1162	ASN
2	C	118	ASN
2	C	136	GLN
2	D	23	GLN
2	D	118	ASN
2	D	136	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z  > 2$
3	ADP	A	1634	-	29,29,29	1.04	2 (6%)	45,45,45	1.85	9 (20%)
3	ADP	B	1634	-	29,29,29	1.04	2 (6%)	45,45,45	1.82	8 (17%)

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
3	ADP	A	1634	-	-	0/16/32/32	0/1/3/3
3	ADP	B	1634	-	-	0/16/32/32	0/1/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1634	ADP	C5-C4	3.07	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1634	ADP	C5-C4	3.04	1.47	1.40
3	A	1634	ADP	C4-N9	-2.76	1.33	1.37
3	B	1634	ADP	C4-N9	-2.59	1.34	1.37

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1634	ADP	N3-C2-N1	-6.36	123.39	128.71
3	B	1634	ADP	N3-C2-N1	-6.16	123.56	128.71
3	B	1634	ADP	N3-C4-N9	5.23	134.87	125.43
3	A	1634	ADP	N3-C4-N9	5.11	134.65	125.43
3	A	1634	ADP	PA-O3A-PB	-3.86	120.35	131.68
3	B	1634	ADP	PA-O3A-PB	-3.76	120.64	131.68
3	B	1634	ADP	C4-C5-N7	-3.56	106.47	109.52
3	A	1634	ADP	C4-C5-N7	-3.40	106.61	109.52
3	B	1634	ADP	C5-C4-N3	-3.18	118.77	125.70
3	A	1634	ADP	C5-C4-N3	-3.05	119.06	125.70
3	B	1634	ADP	O4'-C1'-N9	2.84	111.08	108.44
3	A	1634	ADP	C3'-C2'-C1'	2.62	105.00	100.91
3	A	1634	ADP	C2-N3-C4	2.44	120.97	114.01
3	B	1634	ADP	C2-N3-C4	2.44	120.97	114.01
3	A	1634	ADP	C8-N9-C4	2.34	108.68	106.90
3	B	1634	ADP	C8-N9-C4	2.26	108.62	106.90
3	A	1634	ADP	O4'-C1'-N9	2.01	110.31	108.44

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	625/673 (92%)	0.22	15 (2%) 56 57	37, 67, 111, 134	0
1	B	616/673 (91%)	0.17	9 (1%) 70 71	33, 61, 98, 115	0
2	C	122/147 (82%)	0.22	2 (1%) 68 69	41, 81, 109, 123	0
2	D	122/147 (82%)	0.25	3 (2%) 54 55	43, 70, 93, 119	0
All	All	1485/1640 (90%)	0.20	29 (1%) 64 63	33, 66, 107, 134	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1160	TYR	3.9
1	B	772	ALA	3.5
1	A	1109	PHE	3.4
1	A	1170	TYR	3.4
1	A	1171	VAL	3.3
2	D	66	GLN	3.2
2	C	144	HIS	3.2
2	D	144	HIS	3.1
1	A	1160	TYR	3.1
1	B	848	LEU	3.0
1	A	792	PHE	2.7
1	A	1017	GLU	2.7
2	C	143	HIS	2.5
1	A	639	LEU	2.4
1	A	744	SER	2.4
1	A	746	ALA	2.4
1	A	1163	ALA	2.4
1	B	1001	LEU	2.3
1	B	814	MET	2.3
1	A	1126	ILE	2.3
1	B	1159	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	644	PHE	2.2
1	A	1089	GLN	2.2
2	D	143	HIS	2.1
1	B	1128	SER	2.1
1	B	845	LEU	2.1
1	B	1167	ALA	2.1
1	A	1088	VAL	2.1
1	A	1159	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 ⓘ

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(Å <sup>2</sup> )	Q<0.9
4	ZN	A	1643	1/1	0.19	5.39	54,54,54,54	0
4	ZN	B	1643	1/1	0.21	1.55	55,55,55,55	0
3	ADP	A	1634	27/27	0.20	0.50	34,52,64,84	0
3	ADP	B	1634	27/27	0.18	0.33	29,47,55,62	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.