



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2026 – 12:45 PM EDT

PDB ID : 12UP / pdb\_000012up  
Title : BCL11B ZF2-3 in Complex with a DNA Sequence Observed in the Human Globin Locus Containing Motif TGGCCA (Oligo 4-2)  
Authors : Horton, J.R.; Cheng, X.; Zhou, J.; Lee, J.  
Deposited on : 2026-04-19  
Resolution : 2.83 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

<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  
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

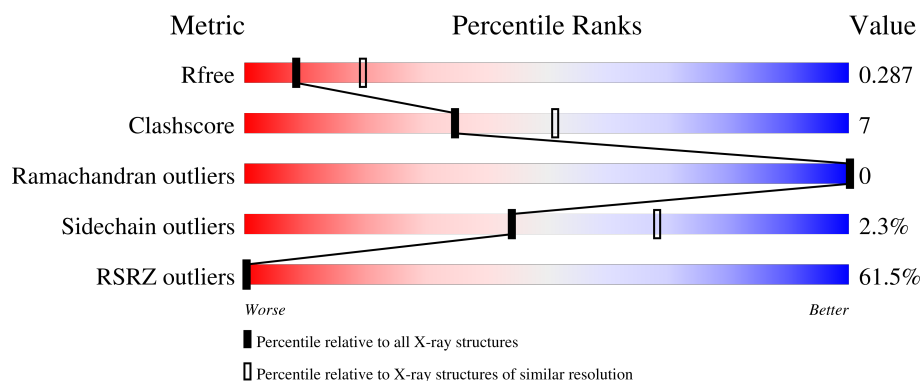
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.83 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	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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	A	66	<div> <div>50%</div> <div>67%</div> <div>14%</div> <div>20%</div> </div>
1	F	66	<div> <div>67%</div> <div>59%</div> <div>20%</div> <div>21%</div> </div>
2	D	13	<div> <div>15%</div> <div>62%</div> <div>38%</div> </div>
2	G	13	<div> <div>38%</div> <div>62%</div> <div>38%</div> </div>
3	E	13	<div> <div>23%</div> <div>69%</div> <div>31%</div> </div>

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Mol	Chain	Length	Quality of chain
3	H	13	<div> <div>69%</div> <div>69%</div> <div>23%</div> <div>8%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 1877 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 B-cell lymphoma/leukemia 11B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	53	Total	C	N	O	S	0	0	0
			417	256	82	73	6			
1	F	52	Total	C	N	O	S	0	0	0
			401	246	80	69	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	418	GLY	-	expression tag	UNP Q9C0K0
A	419	PRO	-	expression tag	UNP Q9C0K0
A	420	LEU	-	expression tag	UNP Q9C0K0
A	421	GLY	-	expression tag	UNP Q9C0K0
A	422	SER	-	expression tag	UNP Q9C0K0
F	418	GLY	-	expression tag	UNP Q9C0K0
F	419	PRO	-	expression tag	UNP Q9C0K0
F	420	LEU	-	expression tag	UNP Q9C0K0
F	421	GLY	-	expression tag	UNP Q9C0K0
F	422	SER	-	expression tag	UNP Q9C0K0

- Molecule 2 is a DNA chain called Strand Top.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	13	Total	C	N	O	P	0	0	0
			262	126	48	76	12			
2	G	13	Total	C	N	O	P	0	0	0
			262	126	48	76	12			

- Molecule 3 is a DNA chain called Strand Bottom.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	13	Total	C	N	O	P	0	0	0
			265	127	50	76	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	12	Total	C	N	O	P	0	0	0
			247	117	45	73	12			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		
4	F	2	Total	Zn	0	0
			2	2		

- Molecule 5 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	2	Total	Br	0	0
			2	2		
5	F	1	Total	Br	0	0
			1	1		
5	H	1	Total	Br	0	0
			1	1		

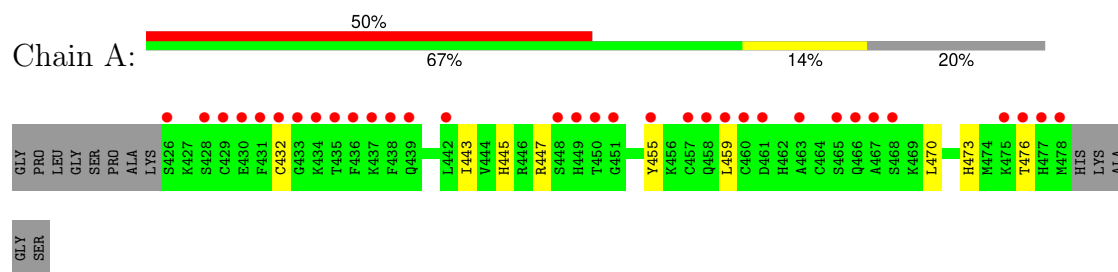
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	O	0	0
			3	3		
6	E	6	Total	O	0	0
			6	6		
6	F	3	Total	O	0	0
			3	3		
6	H	3	Total	O	0	0
			3	3		

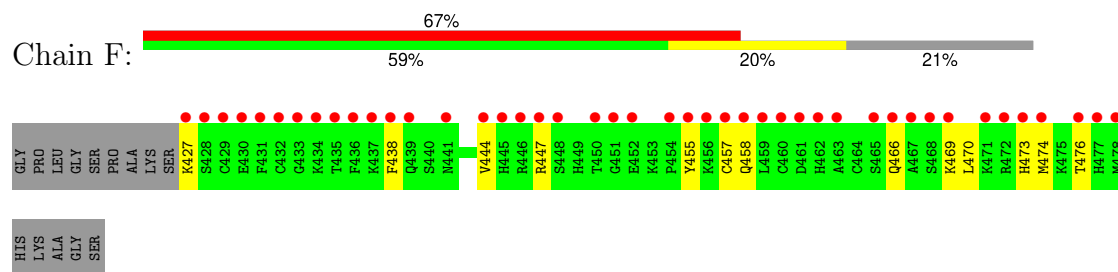
### 3 Residue-property plots

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.

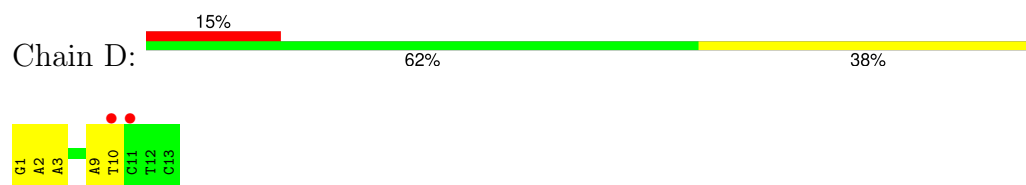
- Molecule 1: B-cell lymphoma/leukemia 11B



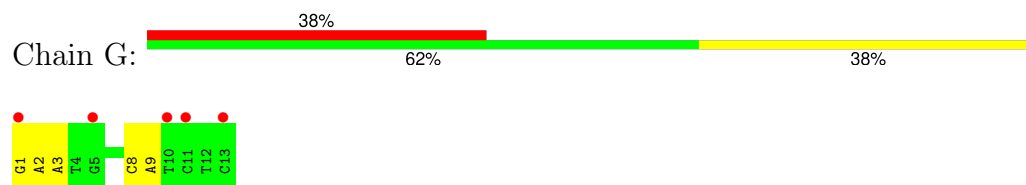
- Molecule 1: B-cell lymphoma/leukemia 11B



- Molecule 2: Strand Top

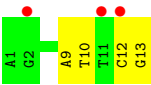


- Molecule 2: Strand Top

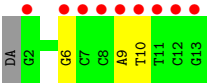


- Molecule 3: Strand Bottom





● Molecule 3: Strand Bottom



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	35.17Å 38.70Å 59.86Å 97.11° 98.65° 99.70°	Depositor
Resolution (Å)	34.15 – 2.83 34.15 – 2.83	Depositor EDS
% Data completeness (in resolution range)	68.5 (34.15-2.83) 68.4 (34.15-2.83)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 2.85Å)	Xtriage
Refinement program	PHENIX 2.0_5885	Depositor
R, $R_{free}$	0.234 , 0.287 0.236 , 0.287	Depositor DCC
$R_{free}$ test set	240 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	8.0	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 44.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	1877	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.53% 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: BR, ZN

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	0.11	0/426	0.31	0/567
1	F	0.10	0/410	0.27	0/547
2	D	0.17	0/293	0.38	0/450
2	G	0.17	0/293	0.40	0/450
3	E	0.21	0/297	0.42	0/457
3	H	0.21	0/276	0.41	0/424
All	All	0.16	0/1995	0.36	0/2895

There are no bond length outliers.

There are no bond angle outliers.

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	A	417	0	396	4	0
1	F	401	0	369	8	0
2	D	262	0	148	4	0
2	G	262	0	148	5	0
3	E	265	0	148	2	0
3	H	247	0	136	2	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	2	0	0	0	0
5	E	2	0	0	0	0
5	F	1	0	0	1	0
5	H	1	0	0	0	0
6	A	3	0	0	0	0
6	E	6	0	0	0	0
6	F	3	0	0	0	0
6	H	3	0	0	0	0
All	All	1877	0	1345	24	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 7.

All (24) 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)
2:D:2:DA:H2''	2:D:3:DA:C8	2.40	0.56
5:F:503:BR:BR	3:H:6:DG:OP2	2.78	0.56
2:G:2:DA:H2''	2:G:3:DA:C8	2.41	0.56
1:A:455:TYR:HB3	1:A:470:LEU:HD22	1.89	0.54
1:F:458:GLN:H	1:F:474:MET:HE1	1.72	0.54
1:F:473:HIS:O	1:F:476:THR:HG22	2.07	0.54
1:A:473:HIS:O	1:A:476:THR:HG22	2.08	0.54
2:D:9:DA:C8	2:D:10:DT:H72	2.42	0.54
1:F:438:PHE:CD1	2:G:1:DG:H2'	2.47	0.50
1:A:432:CYS:SG	1:A:445:HIS:CE1	2.94	0.48
2:D:2:DA:H2''	2:D:3:DA:H8	1.79	0.48
2:G:2:DA:H2''	2:G:3:DA:H8	1.79	0.47
3:E:9:DA:H2'	3:E:10:DT:H71	1.96	0.47
1:A:443:ILE:O	1:A:447:ARG:HG3	2.16	0.45
2:D:1:DG:H2''	2:D:2:DA:C8	2.51	0.45
1:F:455:TYR:HB3	1:F:470:LEU:HD22	1.99	0.44
1:F:457:CYS:HA	1:F:470:LEU:HD11	1.99	0.44
3:H:9:DA:H2'	3:H:10:DT:H71	2.00	0.44
1:F:466:GLN:HB2	1:F:469:LYS:HG2	2.00	0.43
1:F:444:VAL:HA	1:F:447:ARG:HH11	1.83	0.43
2:G:8:DC:H2''	2:G:9:DA:C8	2.54	0.43
2:G:1:DG:H2''	2:G:2:DA:C8	2.55	0.42
3:E:12:DC:H1'	3:E:13:DG:O4'	2.21	0.41
1:F:444:VAL:HA	1:F:447:ARG:NH1	2.37	0.40

There are no symmetry-related clashes.

## 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	
1	A	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
1	F	50/66 (76%)	49 (98%)	1 (2%)	0	100	100
All	All	101/132 (76%)	97 (96%)	4 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	
1	A	46/57 (81%)	45 (98%)	1 (2%)	45	69
1	F	42/57 (74%)	41 (98%)	1 (2%)	43	67
All	All	88/114 (77%)	86 (98%)	2 (2%)	44	68

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	459	LEU
1	F	427	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 8 ligands modelled in this entry, 8 are 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.

No monomer is involved in short contacts.

## 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

### 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	53/66 (80%)	2.34	33 (62%) 0 0	29, 50, 79, 86	0
1	F	52/66 (78%)	3.19	44 (84%) 0 0	38, 64, 94, 118	0
2	D	13/13 (100%)	1.34	2 (15%) 5 4	45, 55, 60, 62	0
2	G	13/13 (100%)	1.73	5 (38%) 1 0	57, 66, 76, 86	0
3	E	13/13 (100%)	1.44	3 (23%) 2 2	47, 54, 60, 62	0
3	H	12/13 (92%)	2.26	9 (75%) 0 0	56, 66, 80, 80	0
All	All	156/184 (84%)	2.41	96 (61%) 0 0	29, 60, 86, 118	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	459	LEU	8.3
1	F	461	ASP	6.4
1	F	457	CYS	5.6
1	F	458	GLN	5.5
1	F	477	HIS	5.4
1	F	465	SER	5.2
1	F	456	LYS	4.8
1	F	471	LYS	4.7
1	A	435	THR	4.6
1	A	431	PHE	4.6
1	F	476	THR	4.6
1	A	434	LYS	4.4
1	F	433	GLY	4.2
1	F	474	MET	4.2
1	A	437	LYS	4.1
1	F	460	CYS	4.0
1	A	461	ASP	4.0
1	A	458	GLN	4.0
3	H	9	DA	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	427	LYS	3.9
1	A	436	PHE	3.7
1	F	435	THR	3.7
3	H	10	DT	3.7
1	F	478	MET	3.7
1	F	447	ARG	3.6
1	A	449	HIS	3.6
1	A	426	SER	3.6
1	A	477	HIS	3.4
1	F	436	PHE	3.3
3	H	11	DT	3.3
1	F	434	LYS	3.3
1	A	448	SER	3.3
1	F	438	PHE	3.2
1	F	428	SER	3.2
1	A	476	THR	3.1
1	F	444	VAL	3.0
1	F	463	ALA	3.0
1	A	430	GLU	3.0
1	F	462	HIS	3.0
1	A	438	PHE	2.9
3	H	12	DC	2.9
1	F	466	GLN	2.9
1	F	473	HIS	2.9
1	A	460	CYS	2.9
1	F	454	PRO	2.8
1	A	450	THR	2.8
1	A	451	GLY	2.8
1	A	459	LEU	2.8
1	A	478	MET	2.8
1	F	431	PHE	2.7
1	F	451	GLY	2.7
1	F	430	GLU	2.7
1	F	445	HIS	2.7
1	F	469	LYS	2.7
1	A	465	SER	2.7
1	F	472	ARG	2.6
1	F	432	CYS	2.6
2	G	13	DC	2.6
1	F	450	THR	2.6
1	F	437	LYS	2.5
1	A	432	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	466	GLN	2.5
1	A	467	ALA	2.5
1	A	442	LEU	2.5
2	G	5	DG	2.5
3	E	12	DC	2.5
1	A	455	TYR	2.5
1	A	433	GLY	2.5
1	F	467	ALA	2.4
1	F	429	CYS	2.4
1	A	428	SER	2.4
1	A	468	SER	2.4
1	F	446	ARG	2.4
1	A	463	ALA	2.4
1	F	455	TYR	2.3
2	G	11	DC	2.3
2	G	10	DT	2.3
1	F	439	GLN	2.3
3	H	7	DC	2.3
1	F	441	ASN	2.2
3	E	11	DT	2.2
1	F	468	SER	2.2
3	H	2	DG	2.2
1	A	475	LYS	2.2
1	F	448	SER	2.1
2	G	1	DG	2.1
3	H	6	DG	2.1
3	H	8	DC	2.1
3	E	2	DG	2.1
3	H	13	DG	2.1
1	A	439	GLN	2.0
1	A	457	CYS	2.0
1	F	452	GLU	2.0
1	A	429	CYS	2.0
2	D	10	DT	2.0
2	D	11	DC	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 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
4	ZN	F	501	1/1	0.84	0.14	102,102,102,102	0
4	ZN	A	501	1/1	0.88	0.09	53,53,53,53	0
5	BR	E	102	1/1	0.89	0.11	76,76,76,76	0
5	BR	E	101	1/1	0.91	0.10	84,84,84,84	0
4	ZN	A	502	1/1	0.95	0.06	58,58,58,58	0
5	BR	F	503	1/1	0.95	0.14	73,73,73,73	0
4	ZN	F	502	1/1	0.96	0.10	34,34,34,34	0
5	BR	H	101	1/1	0.96	0.20	108,108,108,108	0

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

There are no such residues in this entry.