



# wwPDB X-ray Structure Validation Summary Report

Jun 26, 2014 – 09:42 PM EDT

PDB ID : 4P5O  
Title : Structure of an RBX1-UBC12 NEDD8-CUL1-DCN1 complex: a RING-E3-E2 ubiquitin-like protein-substrate intermediate trapped in action  
Authors : Scott, D.C.; Schulman, B.A.  
Deposited on : 2014-03-18  
Resolution : 3.11 Å (reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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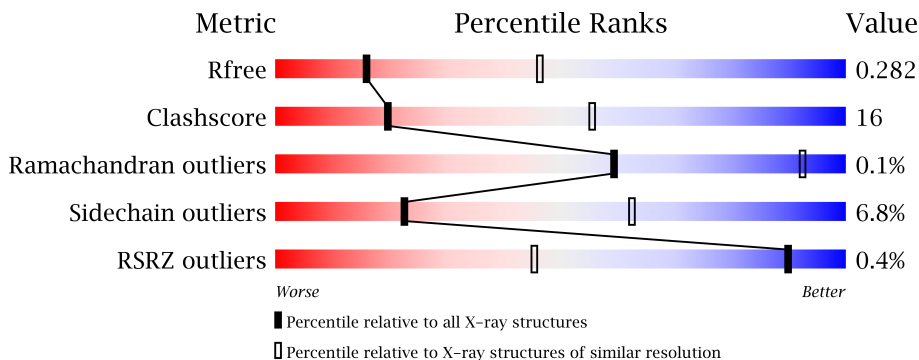
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	<b>FAILED</b>
Xtriage (Phenix)	:	dev-1439
EDS	:	stable23161
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)	:	stable23161

# 1 Overall quality at a glance

The reported resolution of this entry is 3.11 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	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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	368	
1	C	368	
2	B	106	
2	D	106	
3	E	200	
3	F	200	
4	G	189	
4	I	189	
5	H	81	
5	K	81	

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

Mol	Type	Chain	Res	Geometry	Electron density
6	ZN	D	203	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13577 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 Cullin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2631	1671	447	499	14			
1	C	322	Total	C	N	O	S	0	0	0
			2556	1615	436	491	14			

- Molecule 2 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	75	Total	C	N	O	S	0	0	0
			619	393	112	105	9			
2	D	76	Total	C	N	O	S	0	0	0
			624	397	114	104	9			

- Molecule 3 is a protein called DCN1-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	197	Total	C	N	O	S	0	0	0
			1614	1039	264	302	9			
3	F	195	Total	C	N	O	S	0	0	0
			1594	1027	258	300	9			

- Molecule 4 is a protein called NEDD8-conjugating enzyme Ubc12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	169	Total	C	N	O	S	0	0	0
			1374	883	230	254	7			
4	G	171	Total	C	N	O	S	0	0	0
			1384	888	231	258	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	AME	-	expression tag	UNP P61081
I	103	SER	ASN	engineered mutation	UNP P61081
I	111	SER	CYS	engineered mutation	UNP P61081
I	184	HIS	-	expression tag	UNP P61081
G	1	AME	-	expression tag	UNP P61081
G	103	SER	ASN	engineered mutation	UNP P61081
G	111	SER	CYS	engineered mutation	UNP P61081
G	184	HIS	-	expression tag	UNP P61081

- Molecule 5 is a protein called NEDD8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	K	76	Total	C	N	O	S	0	0	0
			591	372	102	115	2			
5	H	76	Total	C	N	O	S	0	0	0
			584	367	102	113	2			

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

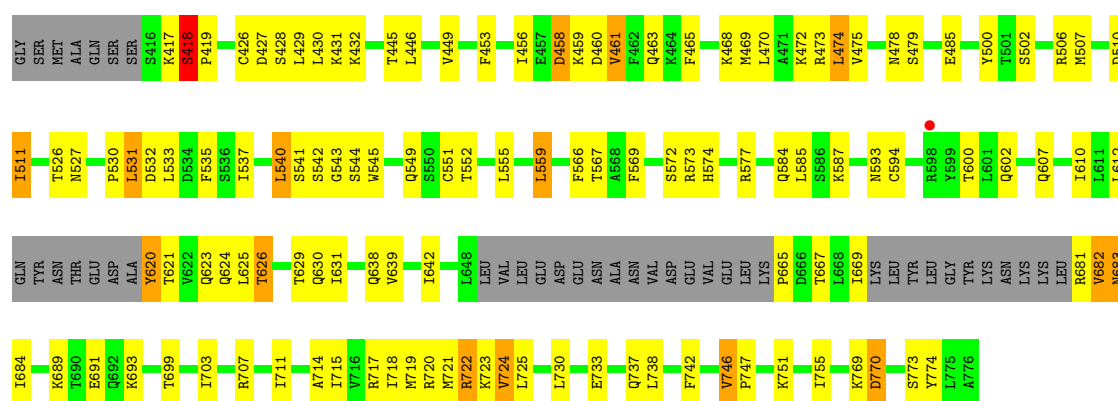
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	3	Total	Zn	0	0
			3	3		
6	D	3	Total	Zn	0	0
			3	3		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

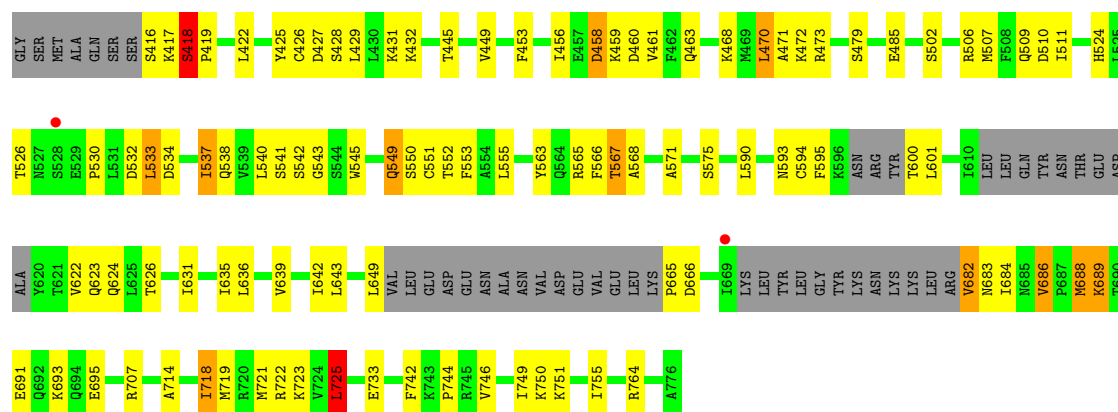
#### • Molecule 1: Cullin-1

Chain A:



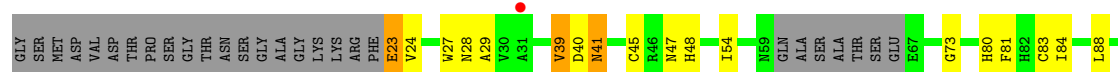
#### • Molecule 1: Cullin-1

Chain C:



#### • Molecule 2: E3 ubiquitin-protein ligase RBX1

Chain B:





- Molecule 2: E3 ubiquitin-protein ligase RBX1

Chain D:



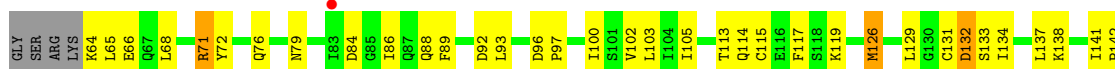
- Molecule 3: DCN1-like protein 1

Chain E:



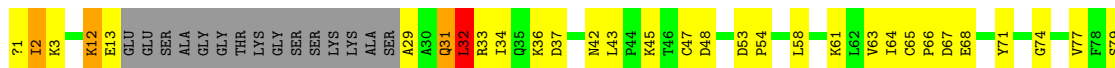
- Molecule 3: DCN1-like protein 1

Chain F:



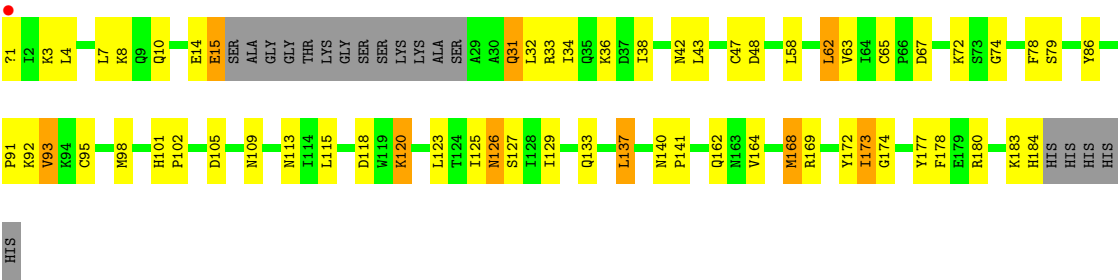
- Molecule 4: NEDD8-conjugating enzyme Ubc12

Chain I:



- Molecule 4: NEDD8-conjugating enzyme Ubc12

Chain G:



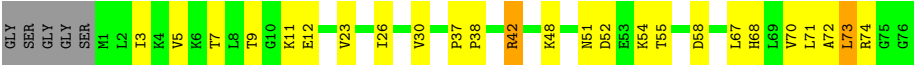
• Molecule 5: NEDD8

Chain K:



• Molecule 5: NEDD8

Chain H:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.11Å 129.61Å 119.94Å 90.00° 111.79° 90.00°	Depositor
Resolution (Å)	42.13 – 3.11 42.13 – 3.11	Depositor EDS
% Data completeness (in resolution range)	99.5 (42.13-3.11) 99.6 (42.13-3.11)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.227 , 0.284 0.225 , 0.282	Depositor DCC
$R_{free}$ test set	2308 reflections (5.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	68.2	Xtriage
Anisotropy	0.907	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 36.5	EDS
Estimated twinning fraction	0.439 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 45490 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13577	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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, AME

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	0.43	0/2670	0.61	0/3587
1	C	0.43	0/2591	0.63	1/3481 (0.0%)
2	B	0.44	0/637	0.60	0/868
2	D	0.42	0/642	0.58	0/874
3	E	0.41	0/1653	0.57	1/2229 (0.0%)
3	F	0.41	0/1633	0.56	1/2204 (0.0%)
4	G	0.51	0/1404	0.65	1/1897 (0.1%)
4	I	0.55	0/1394	0.68	1/1882 (0.1%)
5	H	0.34	0/589	0.57	0/791
5	K	0.36	0/596	0.56	0/800
All	All	0.44	0/13809	0.61	5/18613 (0.0%)

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	A	0	1
1	C	0	1
3	E	0	1
3	F	0	1
All	All	0	4

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	32	LEU	CA-CB-CG	6.95	131.28	115.30
3	F	200	LEU	CA-CB-CG	6.43	130.08	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	200	LEU	CA-CB-CG	5.84	128.74	115.30
1	C	725	LEU	CA-CB-CG	5.53	128.02	115.30
4	G	62	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	418	SER	Peptide
1	C	418	SER	Peptide
3	E	150	GLU	Peptide
3	F	150	GLU	Peptide

## 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	2631	0	2660	104	0
1	C	2556	0	2547	77	0
2	B	619	0	566	17	0
2	D	624	0	575	15	0
3	E	1614	0	1570	54	1
3	F	1594	0	1544	61	0
4	G	1384	0	1361	54	1
4	I	1374	0	1364	48	0
5	H	584	0	603	15	0
5	K	591	0	616	17	0
6	B	3	0	0	0	0
6	D	3	0	0	0	0
All	All	13577	0	13406	433	1

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 16.

The worst 5 of 433 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:720:ARG:NH2	1:A:774:TYR:OH	1.89	1.03
3:E:152:GLY:HA2	3:E:153:ARG:HB2	1.53	0.91
3:E:175:LEU:HD21	3:E:200:LEU:HD13	1.56	0.85
1:C:533:LEU:HD11	2:D:24:VAL:HG22	1.60	0.84
3:F:152:GLY:HA2	3:F:153:ARG:HB2	1.63	0.79

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	Distance(Å)	Clash(Å)
3:E:258:THR:O	4:G:162:GLN:NE2[1_554]	2.14	0.06

## 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	319/368 (87%)	297 (93%)	22 (7%)	0	100	100
1	C	312/368 (85%)	289 (93%)	23 (7%)	0	100	100
2	B	71/106 (67%)	68 (96%)	2 (3%)	1 (1%)	16	58
2	D	72/106 (68%)	69 (96%)	2 (3%)	1 (1%)	16	58
3	E	195/200 (98%)	182 (93%)	13 (7%)	0	100	100
3	F	193/200 (96%)	179 (93%)	14 (7%)	0	100	100
4	G	167/189 (88%)	160 (96%)	7 (4%)	0	100	100
4	I	165/189 (87%)	158 (96%)	7 (4%)	0	100	100
5	H	74/81 (91%)	71 (96%)	3 (4%)	0	100	100
5	K	74/81 (91%)	71 (96%)	3 (4%)	0	100	100
All	All	1642/1888 (87%)	1544 (94%)	96 (6%)	2 (0%)	59	92

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	39	VAL
2	D	39	VAL

### 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	294/339 (87%)	268 (91%)	26 (9%)	14	49
1	C	282/339 (83%)	259 (92%)	23 (8%)	17	53
2	B	66/90 (73%)	61 (92%)	5 (8%)	19	58
2	D	66/90 (73%)	64 (97%)	2 (3%)	53	87
3	E	173/176 (98%)	166 (96%)	7 (4%)	42	82
3	F	171/176 (97%)	163 (95%)	8 (5%)	36	78
4	G	153/170 (90%)	142 (93%)	11 (7%)	21	60
4	I	153/170 (90%)	143 (94%)	10 (6%)	24	65
5	H	62/68 (91%)	57 (92%)	5 (8%)	17	53
5	K	64/68 (94%)	60 (94%)	4 (6%)	25	66
All	All	1484/1686 (88%)	1383 (93%)	101 (7%)	22	62

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	I	140	ASN
1	C	470	LEU
4	G	137	LEU
4	I	165	GLN
5	K	70	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
4	I	140	ASN
1	C	712	GLN
5	K	41	GLN
2	B	41	ASN
1	C	436	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 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	327/368 (88%)	-0.14	1 (0%) 91 53	36, 96, 170, 195	0
1	C	322/368 (87%)	-0.13	2 (0%) 86 36	37, 93, 167, 202	0
2	B	75/106 (70%)	-0.11	1 (1%) 74 19	56, 105, 156, 160	0
2	D	76/106 (71%)	-0.13	0 100 100	54, 108, 138, 157	0
3	E	197/200 (98%)	-0.13	0 100 100	49, 98, 155, 167	0
3	F	195/200 (97%)	-0.16	1 (0%) 88 39	60, 97, 144, 164	0
4	G	171/189 (90%)	-0.12	1 (0%) 86 36	35, 63, 150, 178	0
4	I	169/189 (89%)	-0.21	0 100 100	30, 63, 132, 190	0
5	H	76/81 (93%)	-0.08	0 100 100	75, 123, 155, 168	0
5	K	76/81 (93%)	0.07	1 (1%) 74 19	68, 119, 148, 159	0
All	All	1684/1888 (89%)	-0.13	7 (0%) 90 45	30, 92, 162, 202	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	G	1	AME	3.8
1	C	528	SER	2.8
2	B	31	ALA	2.6
1	A	598	ARG	2.5
5	K	15	ILE	2.2

### 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
6	ZN	D	203	1/1	0.16	2.65	103,103,103,103	0
6	ZN	B	202	1/1	0.23	1.22	82,82,82,82	0
6	ZN	B	203	1/1	0.15	0.69	109,109,109,109	0
6	ZN	B	201	1/1	0.19	0.50	93,93,93,93	0
6	ZN	D	202	1/1	0.18	0.18	78,78,78,78	0
6	ZN	D	201	1/1	0.22	-0.03	103,103,103,103	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.