wwPDB X-ray Structure Validation Summary Report (i)

Oct 25, 2022 – 08:59 pm BST

PDB ID	:	7Z36
Title	:	Crystal structure of the KAP1 tripartite motif in complex with the ZNF93 KRAB domain
Authors	:	Stoll, G.A.; Modis, Y.
Deposited on	:	2022-03-01
Resolution	:	2.80 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

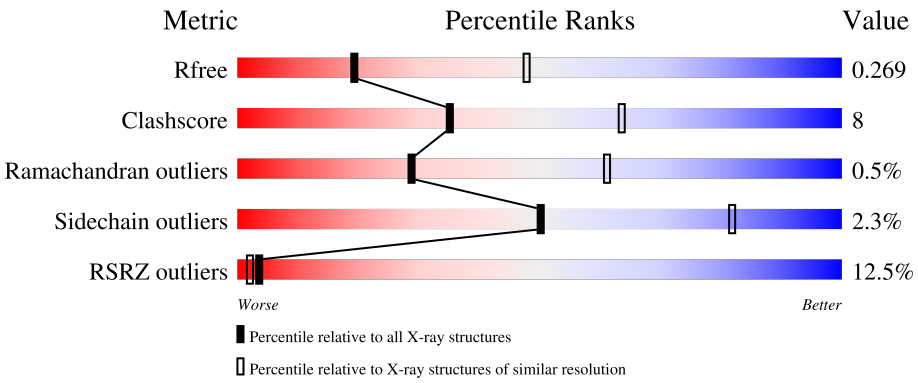
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	482	10% 78% 10% •• 10%
1	B	482	11% 80% 12% 7%
2	C	73	% 56% 5% • 37%
2	S	73	56% 7% • 36%
3	D	70	36% 51% 9% 40%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15589 atoms, of which 7692 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 Endolysin,Transcription intermediary factor 1-beta,Isoform 2 of Transcription intermediary factor 1-beta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	433	6799	2145	3378	626	625	25	0	0	0
1	B	446	6842	2173	3366	632	646	25	0	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P00720
A	2	GLY	-	expression tag	UNP P00720
A	3	SER	-	expression tag	UNP P00720
A	4	SER	-	expression tag	UNP P00720
A	5	HIS	-	expression tag	UNP P00720
A	6	HIS	-	expression tag	UNP P00720
A	7	HIS	-	expression tag	UNP P00720
A	8	HIS	-	expression tag	UNP P00720
A	9	HIS	-	expression tag	UNP P00720
A	10	HIS	-	expression tag	UNP P00720
A	11	SER	-	expression tag	UNP P00720
A	12	GLN	-	expression tag	UNP P00720
A	13	ASP	-	expression tag	UNP P00720
A	14	PRO	-	expression tag	UNP P00720
A	15	ASN	-	expression tag	UNP P00720
A	16	SER	-	expression tag	UNP P00720
A	17	SER	-	expression tag	UNP P00720
A	18	SER	-	expression tag	UNP P00720
A	19	GLU	-	expression tag	UNP P00720
A	20	ASN	-	expression tag	UNP P00720
A	21	LEU	-	expression tag	UNP P00720
A	22	TYR	-	expression tag	UNP P00720
A	23	PHE	-	expression tag	UNP P00720
A	24	GLN	-	expression tag	UNP P00720

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Chain	Residue	Modelled	Actual	Comment	Reference
A	25	GLY	-	expression tag	UNP P00720
A	186	ALA	-	linker	UNP P00720
B	1	MET	-	initiating methionine	UNP P00720
B	2	GLY	-	expression tag	UNP P00720
B	3	SER	-	expression tag	UNP P00720
B	4	SER	-	expression tag	UNP P00720
B	5	HIS	-	expression tag	UNP P00720
B	6	HIS	-	expression tag	UNP P00720
B	7	HIS	-	expression tag	UNP P00720
B	8	HIS	-	expression tag	UNP P00720
B	9	HIS	-	expression tag	UNP P00720
B	10	HIS	-	expression tag	UNP P00720
B	11	SER	-	expression tag	UNP P00720
B	12	GLN	-	expression tag	UNP P00720
B	13	ASP	-	expression tag	UNP P00720
B	14	PRO	-	expression tag	UNP P00720
B	15	ASN	-	expression tag	UNP P00720
B	16	SER	-	expression tag	UNP P00720
B	17	SER	-	expression tag	UNP P00720
B	18	SER	-	expression tag	UNP P00720
B	19	GLU	-	expression tag	UNP P00720
B	20	ASN	-	expression tag	UNP P00720
B	21	LEU	-	expression tag	UNP P00720
B	22	TYR	-	expression tag	UNP P00720
B	23	PHE	-	expression tag	UNP P00720
B	24	GLN	-	expression tag	UNP P00720
B	25	GLY	-	expression tag	UNP P00720
B	186	ALA	-	linker	UNP P00720

- Molecule 2 is a protein called SMARCAD1 CUE1 domain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	C	46	718	221	365	56	74	2	0	0	0
2	S	47	651	208	318	54	70	1	0	0	0

- Molecule 3 is a protein called Zinc finger protein 93.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	D	42	571	200	265	47	57	2	0	0	0

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

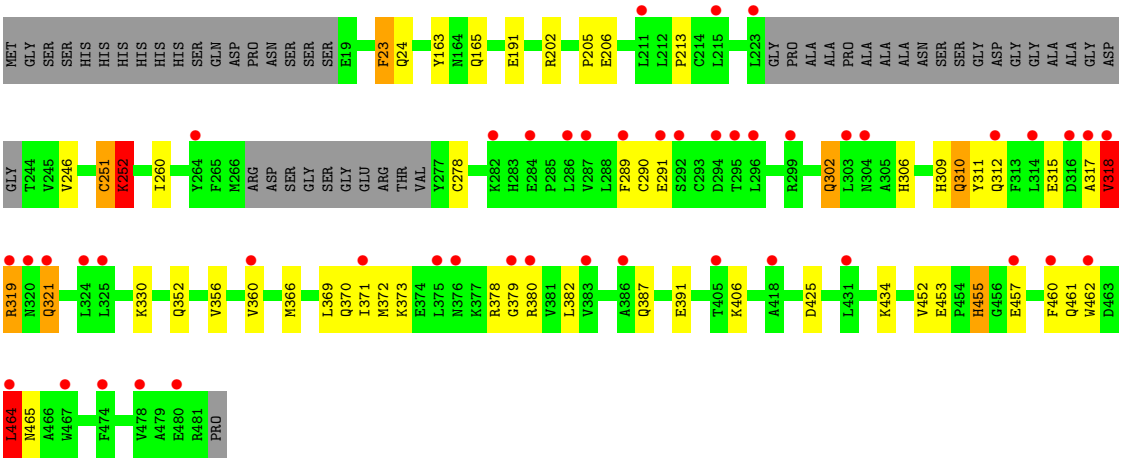
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	A	4	4	4	0	0
4	B	4	4	4	0	0

3 Residue-property plots (i)

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.

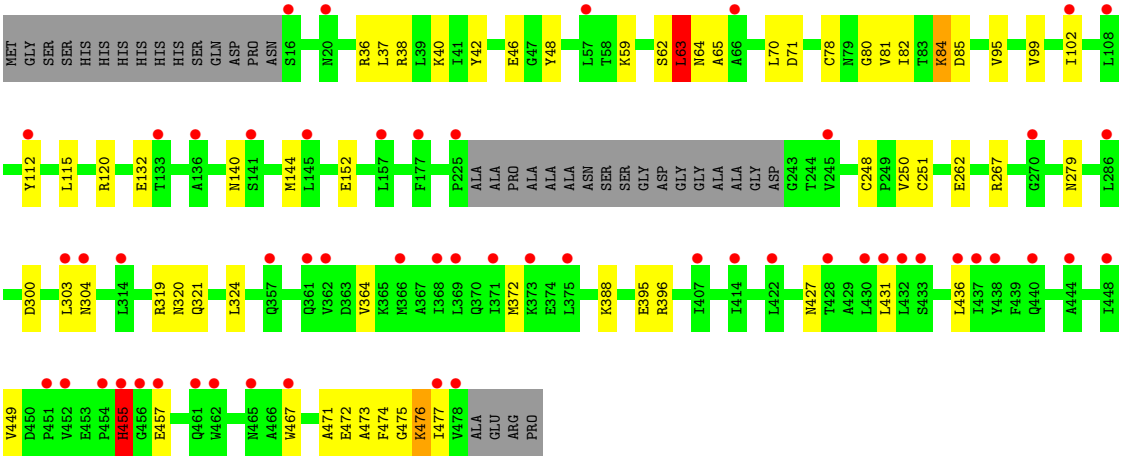
• Molecule 1: Endolysin,Transcription intermediary factor 1-beta,Isoform 2 of Transcription intermediary factor 1-beta

Chain A:



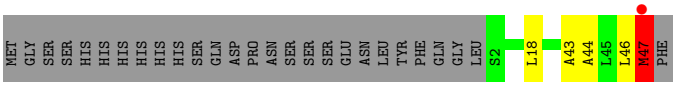
• Molecule 1: Endolysin,Transcription intermediary factor 1-beta,Isoform 2 of Transcription intermediary factor 1-beta

Chain B:



• Molecule 2: SMARCAD1 CUE1 domain

Chain C:

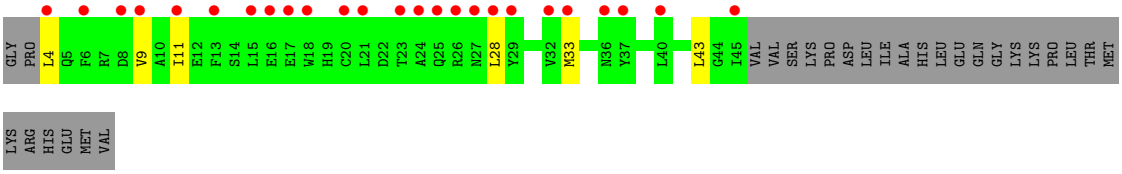


• Molecule 2: SMARCAD1 CUE1 domain

Chain S:

• Molecule 3: Zinc finger protein 93

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	190.28Å 68.58Å 149.11Å 90.00° 114.05° 90.00°	Depositor
Resolution (Å)	63.79 – 2.80 63.79 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.3 (63.79-2.80) 97.3 (63.79-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.75 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.227 , 0.274 0.225 , 0.269	Depositor DCC
R_{free} test set	2224 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å^2)	60.1	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	15589	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.56	2/3477 (0.1%)	0.87	9/4696 (0.2%)
1	B	0.56	3/3535 (0.1%)	0.88	8/4784 (0.2%)
2	C	0.51	0/354	0.89	2/475 (0.4%)
2	S	1.21	2/334 (0.6%)	1.09	5/453 (1.1%)
3	D	0.38	0/311	0.60	0/425
All	All	0.59	7/8011 (0.1%)	0.87	24/10833 (0.2%)

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	B	0	1
2	S	0	1
All	All	0	3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	22	ARG	CG-CD	17.00	1.94	1.51
1	B	63	LEU	CG-CD2	9.72	1.87	1.51
2	S	22	ARG	CD-NE	-7.69	1.33	1.46
1	A	278	CYS	CB-SG	7.36	1.94	1.82
1	B	455	HIS	CA-CB	-6.33	1.40	1.53

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	63	LEU	CB-CG-CD2	-15.95	83.88	111.00
1	A	318	VAL	CG1-CB-CG2	-14.19	88.20	110.90
1	B	63	LEU	CB-CG-CD1	11.21	130.06	111.00
2	S	22	ARG	NE-CZ-NH2	-10.77	114.92	120.30
1	B	455	HIS	N-CA-CB	-10.49	91.72	110.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	319	ARG	Sidechain
1	B	455	HIS	Sidechain
2	S	22	ARG	Sidechain

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	3421	3378	3374	65	1
1	B	3476	3366	3364	54	1
2	C	353	365	365	10	0
2	S	333	318	320	5	0
3	D	306	265	265	10	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
All	All	7897	7692	7688	127	1

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 8.

The worst 5 of 127 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:63:LEU:CD2	1:B:63:LEU:CG	1.87	1.51
2:S:22:ARG:CD	2:S:22:ARG:CG	1.94	1.44
2:C:43:ALA:O	2:C:47:MET:HE3	1.35	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:LEU:CD2	1:B:63:LEU:CD1	2.23	1.15
2:C:43:ALA:O	2:C:47:MET:CE	1.98	1.11

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	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:TYR:HH	1:B:303:LEU:O[1_454]	1.58	0.02

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	427/482 (89%)	415 (97%)	10 (2%)	2 (0%)	29	61
1	B	442/482 (92%)	426 (96%)	13 (3%)	3 (1%)	22	53
2	C	44/73 (60%)	44 (100%)	0	0	100	100
2	S	45/73 (62%)	45 (100%)	0	0	100	100
3	D	40/70 (57%)	40 (100%)	0	0	100	100
All	All	998/1180 (85%)	970 (97%)	23 (2%)	5 (0%)	29	61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	455	HIS
1	B	63	LEU
1	B	80	GLY
1	B	477	ILE
1	A	309	HIS

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	362/415 (87%)	353 (98%)	9 (2%)	47	80
1	B	364/415 (88%)	355 (98%)	9 (2%)	47	80
2	C	40/65 (62%)	39 (98%)	1 (2%)	47	80
2	S	33/65 (51%)	33 (100%)	0	100	100
3	D	28/64 (44%)	28 (100%)	0	100	100
All	All	827/1024 (81%)	808 (98%)	19 (2%)	50	82

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	388	LYS
1	B	455	HIS
2	C	47	MET
1	B	396	ARG
1	A	464	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	387	GLN
2	C	21	GLN
1	A	465	ASN
1	B	64	ASN
1	B	304	ASN

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 monosaccharides 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 (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, 95th 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^2)	Q<0.9
1	A	433/482 (89%)	0.95	46 (10%) 6 3	27, 55, 121, 157	0
1	B	446/482 (92%)	0.96	55 (12%) 4 2	27, 66, 116, 154	0
2	C	46/73 (63%)	0.45	1 (2%) 62 52	34, 50, 87, 111	0
2	S	47/73 (64%)	0.36	0 100 100	60, 80, 141, 151	0
3	D	42/70 (60%)	2.25	25 (59%) 0 0	81, 104, 120, 126	0
All	All	1014/1180 (85%)	0.96	127 (12%) 3 2	27, 64, 121, 157	0

The worst 5 of 127 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	33	MET	8.7
1	A	296	LEU	8.3
1	A	317	ALA	7.0
1	A	314	LEU	7.0
1	A	320	ASN	6.3

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 monosaccharides 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, 95th 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(Å^2)	Q<0.9
4	ZN	A	503	1/1	0.43	0.13	138,138,138,138	0
4	ZN	A	504	1/1	0.85	0.10	132,132,132,132	0
4	ZN	B	503	1/1	0.94	0.16	91,91,91,91	0
4	ZN	B	504	1/1	0.94	0.20	74,74,74,74	0
4	ZN	B	502	1/1	0.96	0.26	39,39,39,39	0
4	ZN	B	501	1/1	0.97	0.28	39,39,39,39	0
4	ZN	A	501	1/1	0.97	0.22	66,66,66,66	0
4	ZN	A	502	1/1	0.98	0.22	77,77,77,77	0

6.5 Other polymers (i)

There are no such residues in this entry.