



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:38 AM GMT

PDB ID : 4A4Z  
Title : CRYSTAL STRUCTURE OF THE S. CEREVISIAE DEXH HELICASE SKI2  
BOUND TO AMPPNP  
Authors : Halbach, F.; Rode, M.; Conti, E.  
Deposited on : 2011-10-20  
Resolution : 2.40 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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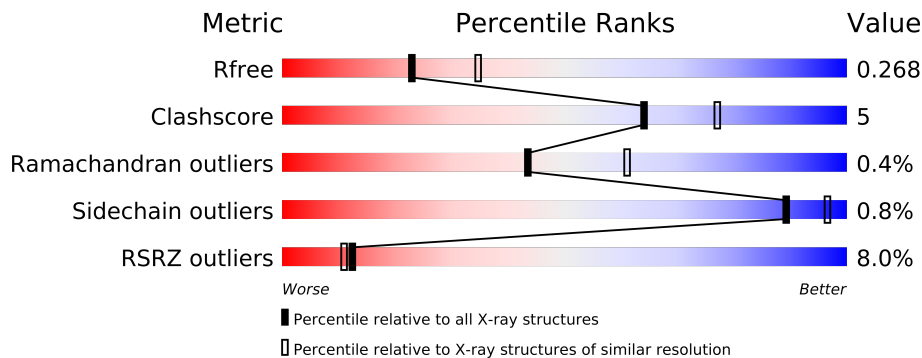
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.40 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	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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	997	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	EDO	A	2289	-	X
3	EDO	A	2291	-	X
3	EDO	A	2292	-	X

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 6683 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.

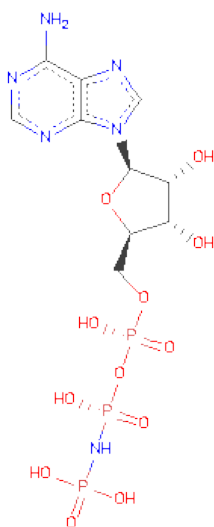
- Molecule 1 is a protein called ANTIVIRAL HELICASE SKI2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	874	6503	4155	1123	1196	29	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

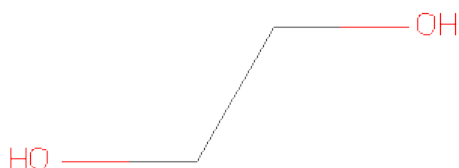
Chain	Residue	Modelled	Actual	Comment	Reference
A	291	GLY	-	EXPRESSION TAG	UNP P35207
A	292	PRO	-	EXPRESSION TAG	UNP P35207
A	293	ASP	-	EXPRESSION TAG	UNP P35207
A	294	SER	-	EXPRESSION TAG	UNP P35207
A	295	MET	-	EXPRESSION TAG	UNP P35207

- Molecule 2 is PHOSPHOAMINOPHOSPHONICACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

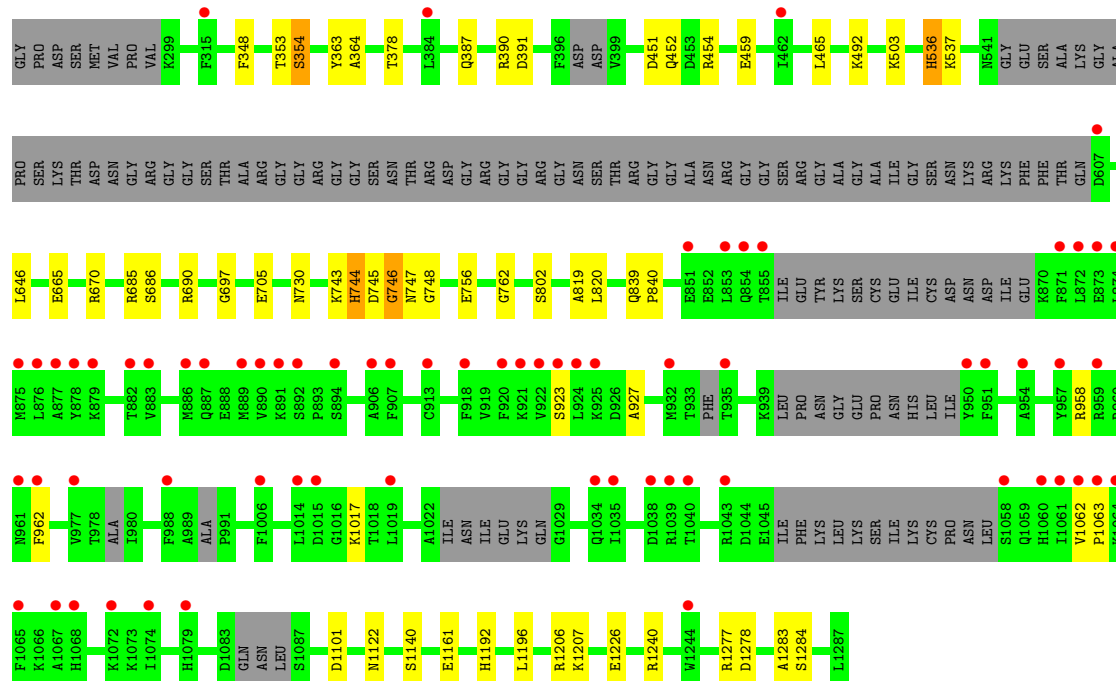
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	133	Total	O	0	0
			133	133		

### 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: ANTIVIRAL HELICASE SKI2

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.79Å 118.55Å 129.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.43 – 2.40 51.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.43-2.40) 99.7 (51.00-2.40)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.75 (at 2.39Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.1.743)	Depositor
R, $R_{free}$	0.238 , 0.275 0.228 , 0.268	Depositor DCC
$R_{free}$ test set	2559 reflections (5.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.3	Xtriage
Anisotropy	0.535	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 46.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 50441 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6683	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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: ANP, EDO

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	0.23	0/6620	0.40	0/8997

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	6503	0	39	36	0
2	A	31	0	0	0	0
3	A	16	0	24	0	0
4	A	133	0	0	9	0
All	All	6683	0	63	36	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 5.

All (36) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:387:GLN:NE2	1:A:730:ASN:OD1	2.16	0.78
1:A:1206:ARG:O	4:A:2121:HOH:O	2.06	0.72
1:A:1140:SER:OG	4:A:2108:HOH:O	2.07	0.71
1:A:819:ALA:O	4:A:2092:HOH:O	2.09	0.70
1:A:454:ARG:NH2	1:A:1122:ASN:O	2.29	0.65
1:A:1226:GLU:OE1	4:A:2123:HOH:O	2.15	0.65
1:A:762:GLY:O	4:A:2079:HOH:O	2.15	0.63
1:A:745:ASP:O	1:A:748:GLY:N	2.33	0.61
1:A:670:ARG:NH1	1:A:1283:ALA:O	2.34	0.61
1:A:353:THR:O	1:A:354:SER:OG	2.18	0.61
1:A:390:ARG:NH2	1:A:391:ASP:OD1	2.38	0.57
1:A:665:GLU:OE1	1:A:685:ARG:NH2	2.40	0.55
1:A:353:THR:O	1:A:354:SER:CB	2.55	0.54
1:A:451:ASP:OD1	1:A:452:GLN:N	2.44	0.51
1:A:745:ASP:O	1:A:747:ASN:N	2.45	0.50
1:A:503:LYS:O	4:A:2027:HOH:O	2.19	0.50
1:A:820:LEU:N	4:A:2091:HOH:O	2.45	0.49
1:A:743:LYS:NZ	1:A:756:GLU:OE2	2.46	0.48
1:A:378:THR:OG1	4:A:2007:HOH:O	2.20	0.48
1:A:744:HIS:C	1:A:744:HIS:ND1	2.66	0.48
1:A:1206:ARG:NH1	4:A:2112:HOH:O	2.47	0.47
1:A:705:GLU:OE2	1:A:1284:SER:OG	2.33	0.47
1:A:697:GLY:O	1:A:1240:ARG:NH2	2.49	0.46
1:A:1161:GLU:O	1:A:1207:LYS:NZ	2.50	0.44
1:A:536:HIS:CG	1:A:537:LYS:N	2.85	0.44
1:A:958:ARG:O	1:A:962:PHE:N	2.51	0.43
1:A:1277:ARG:NH1	1:A:1278:ASP:OD2	2.52	0.43
1:A:465:LEU:O	1:A:492:LYS:NZ	2.52	0.43
1:A:363:TYR:O	1:A:364:ALA:C	2.57	0.42
1:A:839:GLN:CB	1:A:840:PRO:CD	2.98	0.42
1:A:646:LEU:O	1:A:690:ARG:NH2	2.53	0.41
1:A:745:ASP:O	1:A:746:GLY:C	2.57	0.41
1:A:923:SER:O	1:A:927:ALA:N	2.54	0.40
1:A:1062:VAL:HB	1:A:1063:PRO:CD	2.52	0.40
1:A:459:GLU:OE1	1:A:802:SER:OG	2.39	0.40
1:A:1101:ASP:OD2	1:A:1192:HIS:NE2	2.55	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	852/997 (86%)	801 (94%)	48 (6%)	3 (0%)	43 61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	354	SER
1	A	746	GLY
1	A	1017	LYS

### 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	623/881 (71%)	618 (99%)	5 (1%)	89 96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	348	PHE
1	A	536	HIS
1	A	686	SER
1	A	744	HIS
1	A	1196	LEU

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

### 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 ⓘ

5 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	ANP	A	2288	-	33,33,33	1.79	8 (24%)	51,52,52	2.67	17 (33%)
3	EDO	A	2289	-	3,3,3	0.53	0	2,2,2	0.35	0
3	EDO	A	2290	-	3,3,3	0.53	0	2,2,2	0.36	0
3	EDO	A	2291	-	3,3,3	0.54	0	2,2,2	0.33	0
3	EDO	A	2292	-	3,3,3	0.53	0	2,2,2	0.40	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	ANP	A	2288	-	-	1/18/38/38	0/1/3/3
3	EDO	A	2289	-	-	0/1/1/1	0/0/0/0
3	EDO	A	2290	-	-	0/1/1/1	0/0/0/0
3	EDO	A	2291	-	-	0/1/1/1	0/0/0/0
3	EDO	A	2292	-	-	0/1/1/1	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2288	ANP	C2'-C1'	-3.72	1.48	1.53
2	A	2288	ANP	PB-N3B	3.29	1.67	1.64
2	A	2288	ANP	PB-O1B	3.27	1.50	1.46
2	A	2288	ANP	C6-N6	3.14	1.45	1.35
2	A	2288	ANP	PG-O1G	2.57	1.49	1.46
2	A	2288	ANP	PG-N3B	2.55	1.66	1.64
2	A	2288	ANP	O3'-C3'	-2.16	1.37	1.43
2	A	2288	ANP	C2-N3	2.06	1.36	1.32

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2288	ANP	PB-N3B-PG	-10.36	112.65	130.07
2	A	2288	ANP	N3-C2-N1	-8.72	121.42	128.71
2	A	2288	ANP	N3-C4-N9	4.84	134.17	125.43
2	A	2288	ANP	O3G-PG-O1G	-4.01	103.32	113.60
2	A	2288	ANP	C8-N9-C4	3.80	109.80	106.90
2	A	2288	ANP	PA-O3A-PB	-3.61	119.47	131.81
2	A	2288	ANP	O2B-PB-O1B	-3.54	101.70	109.89
2	A	2288	ANP	O2G-PG-O1G	-3.40	104.87	113.60
2	A	2288	ANP	O3G-PG-N3B	3.03	114.83	106.61
2	A	2288	ANP	O2G-PG-N3B	2.83	114.30	106.61
2	A	2288	ANP	C5-C4-N3	-2.73	119.77	125.70
2	A	2288	ANP	C4'-O4'-C1'	-2.41	107.13	109.75
2	A	2288	ANP	C4-C5-N7	-2.36	107.50	109.52
2	A	2288	ANP	N7-C8-N9	-2.34	107.73	114.36
2	A	2288	ANP	C2-N3-C4	2.18	120.22	114.01
2	A	2288	ANP	C3'-C2'-C1'	2.08	104.17	100.91
2	A	2288	ANP	O3A-PB-N3B	2.08	112.35	106.59

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2288	ANP	O1G-PG-N3B-PB

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	874/997 (87%)	0.40	70 (8%) 12 11	27, 59, 136, 182	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	876	LEU	8.0
1	A	1058	SER	7.1
1	A	1061	ILE	6.7
1	A	872	LEU	6.3
1	A	871	PHE	5.9
1	A	1014	LEU	5.8
1	A	1063	PRO	5.8
1	A	892	SER	4.6
1	A	924	LEU	4.5
1	A	935	THR	4.2
1	A	1062	VAL	4.2
1	A	961	ASN	4.2
1	A	977	VAL	4.0
1	A	1065	PHE	4.0
1	A	873	GLU	3.9
1	A	894	SER	3.9
1	A	855	THR	3.9
1	A	1039	ARG	3.9
1	A	878	TYR	3.6
1	A	315	PHE	3.5
1	A	875	MET	3.4
1	A	874	LEU	3.4
1	A	854	GLN	3.4
1	A	922	VAL	3.4
1	A	920	PHE	3.3
1	A	951	PHE	3.3
1	A	882	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	962	PHE	3.3
1	A	1060	HIS	3.3
1	A	932	MET	3.3
1	A	607	ASP	3.3
1	A	1067	ALA	3.3
1	A	889	MET	3.1
1	A	1064	LYS	3.1
1	A	879	LYS	3.0
1	A	851	GLU	3.0
1	A	1035	ILE	2.9
1	A	853	LEU	2.8
1	A	907	PHE	2.8
1	A	954	ALA	2.8
1	A	1068	HIS	2.8
1	A	877	ALA	2.7
1	A	913	CYS	2.7
1	A	886	MET	2.7
1	A	918	PHE	2.7
1	A	923	SER	2.6
1	A	887	GLN	2.6
1	A	384	LEU	2.6
1	A	959	ARG	2.5
1	A	890	VAL	2.5
1	A	925	LYS	2.5
1	A	950	TYR	2.5
1	A	883	VAL	2.4
1	A	957	TYR	2.4
1	A	1015	ASP	2.4
1	A	1019	LEU	2.4
1	A	1006	PHE	2.4
1	A	988	PHE	2.3
1	A	921	LYS	2.3
1	A	1038	ASP	2.3
1	A	891	LYS	2.3
1	A	906	ALA	2.2
1	A	462	ILE	2.2
1	A	1040	THR	2.2
1	A	1074	ILE	2.2
1	A	1043	ARG	2.2
1	A	1072	LYS	2.1
1	A	1079	HIS	2.1
1	A	1034	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1244	TRP	2.1

## 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
3	EDO	A	2291	4/4	0.41	8.31	72,72,73,73	0
3	EDO	A	2289	4/4	0.24	3.11	58,58,59,59	0
3	EDO	A	2292	4/4	0.21	2.85	56,56,56,56	0
3	EDO	A	2290	4/4	0.26	1.83	55,55,56,56	0
2	ANP	A	2288	31/31	0.18	0.78	75,82,85,87	3

## 6.5 Other polymers ⓘ

There are no such residues in this entry.