



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 11:38 pm GMT

PDB ID : 2B52  
Title : Human cyclin dependent kinase 2 (CDK2) complexed with DPH-042562  
Authors : Muckelbauer, J.  
Deposited on : 2005-09-27  
Resolution : 1.88 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

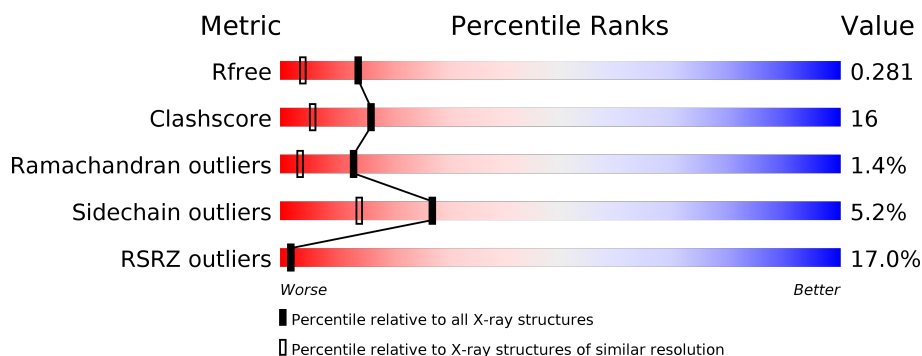
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.88 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))
$R_{free}$	100719	7505 (1.90-1.86)
Clashscore	112137	8369 (1.90-1.86)
Ramachandran outliers	110173	8279 (1.90-1.86)
Sidechain outliers	110143	8280 (1.90-1.86)
RSRZ outliers	101464	7571 (1.90-1.86)

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. 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	298	

## 2 Entry composition [i](#)

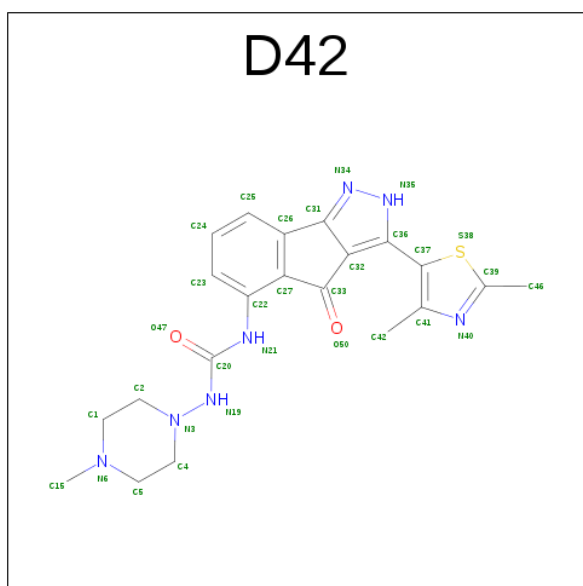
There are 3 unique types of molecules in this entry. The entry contains 2368 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cell division protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2277	1482	387	400	8			

- Molecule 2 is 1-(3-(2,4-DIMETHYLTHIAZOL-5-YL)-4-OXO-2,4-DIHYDROINDENO[1,2-C]PYRAZOL-5-YL)-3-(4-METHYLPIPERAZIN-1-YL)UREA (three-letter code: D42) (formula: C<sub>21</sub>H<sub>23</sub>N<sub>7</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			31	21	7	2	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	60	Total	O	0	0
			60	60		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.03Å 72.01Å 53.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.71 – 1.88 18.71 – 1.88	Depositor EDS
% Data completeness (in resolution range)	86.8 (18.71-1.88) 96.0 (18.71-1.88)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.61 (at 1.89Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, $R_{free}$	0.219 , 0.275 0.228 , 0.281	Depositor DCC
$R_{free}$ test set	1753 reflections (8.53%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.7	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 60.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2368	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: D42

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	0.37	0/2334	0.58	0/3162

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

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	2277	0	2329	75	0
2	A	31	0	23	3	0
3	A	60	0	0	4	0
All	All	2368	0	2352	75	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 16.

All (75) 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:A:1:MET:HE3	1:A:3:ASN:H	1.34	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:VAL:HG21	1:A:134:LEU:HD12	1.65	0.78
1:A:210:ASP:O	1:A:214:ARG:HG3	1.85	0.77
1:A:128:LEU:HD21	1:A:143:LEU:CD2	2.22	0.70
1:A:128:LEU:HD21	1:A:143:LEU:HD22	1.74	0.70
1:A:15:TYR:HB2	1:A:33:LYS:NZ	2.09	0.67
1:A:56:LYS:NZ	1:A:56:LYS:HB3	2.09	0.67
1:A:60:HIS:HD2	1:A:62:ASN:H	1.42	0.64
1:A:60:HIS:CD2	1:A:62:ASN:H	2.16	0.64
1:A:41:THR:OG1	1:A:75:LYS:HD2	1.97	0.64
1:A:145:ASP:OD2	2:A:299:D42:H22	2.00	0.61
1:A:64:VAL:HG21	1:A:144:ALA:HB2	1.82	0.60
1:A:261:SER:O	1:A:265:GLN:HG3	2.01	0.60
1:A:43:GLY:HA2	1:A:74:ASN:HD22	1.65	0.60
1:A:131:GLN:NE2	1:A:131:GLN:H	2.00	0.60
1:A:43:GLY:HA2	1:A:74:ASN:ND2	2.17	0.58
1:A:290:THR:O	1:A:292:PRO:HD3	2.04	0.58
1:A:47:THR:O	1:A:51:GLU:HG2	2.04	0.58
1:A:9:LYS:HG2	1:A:19:TYR:CE1	2.38	0.58
1:A:1:MET:HE3	1:A:3:ASN:N	2.11	0.58
1:A:86:ASP:OD2	2:A:299:D42:H463	2.04	0.57
1:A:84:HIS:HB3	1:A:298:LEU:HD22	1.85	0.56
1:A:85:GLN:HE21	1:A:90:PHE:HB2	1.70	0.56
1:A:64:VAL:CG2	1:A:134:LEU:HD12	2.35	0.56
1:A:25:LEU:CD1	1:A:26:THR:HG23	2.37	0.55
1:A:16:GLY:HA2	1:A:36:ARG:HD2	1.88	0.55
1:A:86:ASP:OD1	1:A:88:LYS:HB3	2.07	0.54
1:A:1:MET:HG3	1:A:70:ILE:HD13	1.88	0.54
1:A:199:ARG:HD2	3:A:344:HOH:O	2.07	0.54
1:A:175:LEU:HD21	1:A:212:LEU:HD21	1.91	0.53
1:A:87:LEU:O	1:A:91:MET:HG3	2.08	0.53
1:A:247:ASP:O	1:A:251:VAL:HG23	2.09	0.53
1:A:146:PHE:HB2	1:A:148:LEU:HD21	1.92	0.51
1:A:23:ASN:OD1	1:A:25:LEU:HG	2.10	0.51
1:A:56:LYS:HZ2	1:A:56:LYS:HB3	1.75	0.51
1:A:103:LEU:HD11	1:A:294:PRO:HB3	1.93	0.51
1:A:178:LYS:HD3	1:A:178:LYS:H	1.76	0.50
1:A:88:LYS:HE2	3:A:357:HOH:O	2.11	0.50
1:A:122:ARG:HE	1:A:122:ARG:HA	1.76	0.50
1:A:129:LYS:HG2	1:A:132:ASN:ND2	2.27	0.49
1:A:297:ARG:NE	1:A:297:ARG:HA	2.27	0.49
1:A:15:TYR:HB2	1:A:33:LYS:HZ3	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:LYS:HD3	1:A:178:LYS:N	2.28	0.49
1:A:15:TYR:HB2	1:A:33:LYS:HZ1	1.77	0.48
1:A:84:HIS:CD2	1:A:298:LEU:HD13	2.49	0.48
1:A:162:GLU:O	1:A:163:VAL:HG13	2.14	0.47
1:A:230:VAL:O	1:A:233:MET:HG2	2.14	0.47
1:A:297:ARG:HA	1:A:297:ARG:CZ	2.44	0.47
1:A:125:HIS:O	1:A:126:ARG:HB2	2.14	0.47
1:A:62:ASN:ND2	1:A:110:GLN:HB3	2.29	0.47
1:A:273:LYS:HD2	3:A:322:HOH:O	2.16	0.46
1:A:83:LEU:O	2:A:299:D42:N35	2.43	0.46
1:A:12:GLU:HA	1:A:17:VAL:HA	1.97	0.45
1:A:294:PRO:HG2	1:A:296:LEU:HG	1.99	0.45
1:A:64:VAL:CG2	1:A:144:ALA:HB2	2.44	0.45
1:A:69:VAL:HG13	1:A:69:VAL:O	2.16	0.44
1:A:34:LYS:HG3	1:A:77:TYR:CE1	2.53	0.44
1:A:43:GLY:O	1:A:44:VAL:HB	2.18	0.43
1:A:9:LYS:HG2	1:A:19:TYR:CD1	2.53	0.43
1:A:231:THR:HA	1:A:236:TYR:CD2	2.53	0.43
1:A:130:PRO:HB2	1:A:131:GLN:HE21	1.82	0.43
1:A:174:LEU:HD11	1:A:211:GLN:HG3	2.01	0.43
1:A:224:GLU:OE2	1:A:231:THR:HG23	2.19	0.43
1:A:119:HIS:CE1	1:A:182:THR:HB	2.54	0.42
1:A:35:ILE:HD11	1:A:78:LEU:HD12	2.00	0.42
1:A:3:ASN:HB3	1:A:25:LEU:HD23	2.01	0.42
1:A:174:LEU:CB	1:A:212:LEU:HD13	2.48	0.42
1:A:203:PHE:CZ	1:A:219:LEU:HD21	2.54	0.42
1:A:230:VAL:HG13	1:A:231:THR:N	2.35	0.41
1:A:66:LEU:HD13	1:A:80:PHE:CE1	2.56	0.41
1:A:167:TRP:CD1	1:A:204:PRO:HA	2.55	0.41
1:A:46:SER:HA	1:A:49:ILE:HG12	2.02	0.41
1:A:137:THR:HA	1:A:296:LEU:HD12	2.03	0.40
1:A:1:MET:HB2	3:A:351:HOH:O	2.21	0.40
1:A:7:VAL:HG21	1:A:22:ARG:HB2	2.03	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	277/298 (93%)	258 (93%)	15 (5%)	4 (1%)	13 3

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	GLU
1	A	163	VAL
1	A	6	LYS
1	A	44	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	250/263 (95%)	237 (95%)	13 (5%)	27 14

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	12	GLU
1	A	25	LEU
1	A	76	LEU
1	A	89	LYS
1	A	103	LEU
1	A	131	GLN

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Mol	Chain	Res	Type
1	A	162	GLU
1	A	178	LYS
1	A	202	LEU
1	A	219	LEU
1	A	268	HIS
1	A	287	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	60	HIS
1	A	74	ASN
1	A	84	HIS
1	A	85	GLN
1	A	113	GLN
1	A	131	GLN
1	A	268	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	D42	A	299	-	31,35,35	3.61	16 (51%)	31,52,52	4.37	16 (51%)

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	D42	A	299	-	-	0/8/34/34	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	299	D42	C27-C33	-2.70	1.46	1.49
2	A	299	D42	C32-C33	-2.67	1.46	1.49
2	A	299	D42	C46-C39	2.01	1.52	1.49
2	A	299	D42	C39-S38	2.95	1.82	1.73
2	A	299	D42	C27-C22	3.17	1.47	1.41
2	A	299	D42	C31-N34	3.47	1.41	1.34
2	A	299	D42	C36-N35	3.49	1.41	1.34
2	A	299	D42	C32-C31	3.53	1.45	1.41
2	A	299	D42	C32-C36	4.08	1.45	1.41
2	A	299	D42	C25-C26	4.36	1.47	1.39
2	A	299	D42	C26-C27	4.68	1.47	1.41
2	A	299	D42	C24-C23	4.72	1.47	1.38
2	A	299	D42	C24-C25	4.84	1.48	1.38
2	A	299	D42	C23-C22	5.10	1.48	1.39
2	A	299	D42	N35-N34	7.91	1.52	1.37
2	A	299	D42	N19-N3	11.13	1.51	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	299	D42	C27-C22-N21	-4.51	112.13	118.80
2	A	299	D42	C27-C26-C31	-3.85	105.03	108.55
2	A	299	D42	O50-C33-C27	-3.24	124.75	127.68
2	A	299	D42	C32-C36-N35	-2.63	104.28	108.41
2	A	299	D42	C26-C27-C33	2.36	111.16	108.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	299	D42	C36-C32-C31	2.37	108.04	104.00
2	A	299	D42	C4-N3-C2	2.45	113.15	110.16
2	A	299	D42	O50-C33-C32	2.56	130.00	127.68
2	A	299	D42	C31-C32-C33	2.61	109.27	107.78
2	A	299	D42	N19-C20-N21	2.72	118.97	113.34
2	A	299	D42	C46-C39-S38	3.09	124.27	120.12
2	A	299	D42	C32-C31-N34	3.11	113.28	108.41
2	A	299	D42	C5-N6-C1	4.23	115.12	109.47
2	A	299	D42	C2-N3-N19	5.12	114.43	110.11
2	A	299	D42	C15-N6-C5	5.48	118.93	110.67
2	A	299	D42	C4-N3-N19	19.71	126.72	110.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	299	D42	3	0

## 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	283/298 (94%)	0.96	48 (16%) 2 2	15, 38, 73, 87	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	41	THR	7.5
1	A	15	TYR	7.1
1	A	44	VAL	6.8
1	A	36	ARG	6.8
1	A	161	HIS	5.8
1	A	25	LEU	5.8
1	A	14	THR	5.7
1	A	163	VAL	5.7
1	A	43	GLY	5.5
1	A	148	LEU	5.3
1	A	45	PRO	4.8
1	A	164	VAL	4.7
1	A	47	THR	3.9
1	A	298	LEU	3.9
1	A	96	LEU	3.9
1	A	42	GLU	3.9
1	A	12	GLU	3.7
1	A	54	LEU	3.7
1	A	73	GLU	3.6
1	A	46	SER	3.6
1	A	162	GLU	3.6
1	A	78	LEU	3.3
1	A	13	GLY	3.3
1	A	74	ASN	3.2
1	A	297	ARG	3.2
1	A	50	ARG	3.1
1	A	75	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	26	THR	3.0
1	A	51	GLU	2.8
1	A	32	LEU	2.7
1	A	49	ILE	2.7
1	A	248	PHE	2.5
1	A	57	GLU	2.5
1	A	72	THR	2.5
1	A	19	TYR	2.4
1	A	293	VAL	2.4
1	A	287	GLN	2.4
1	A	295	HIS	2.4
1	A	21	ALA	2.3
1	A	77	TYR	2.2
1	A	240	PHE	2.2
1	A	146	PHE	2.2
1	A	246	GLN	2.2
1	A	1	MET	2.1
1	A	122	ARG	2.1
1	A	149	ALA	2.0
1	A	147	GLY	2.0
1	A	10	ILE	2.0

## 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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	D42	A	299	31/31	0.75	0.20	0.20	42,47,56,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.