



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 06:06 pm GMT

PDB ID : 2HYD  
Title : Multidrug ABC transporter SAV1866  
Authors : Dawson, R.J.P.; Locher, K.P.  
Deposited on : 2006-08-05  
Resolution : 3.00 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](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

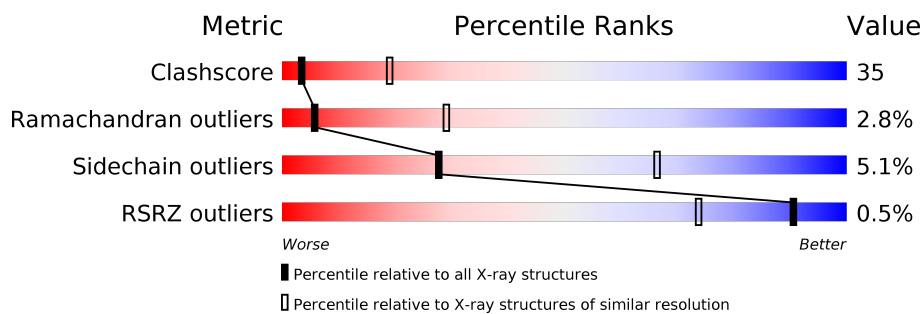
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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	578	
1	B	578	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NA	B	910	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9240 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.

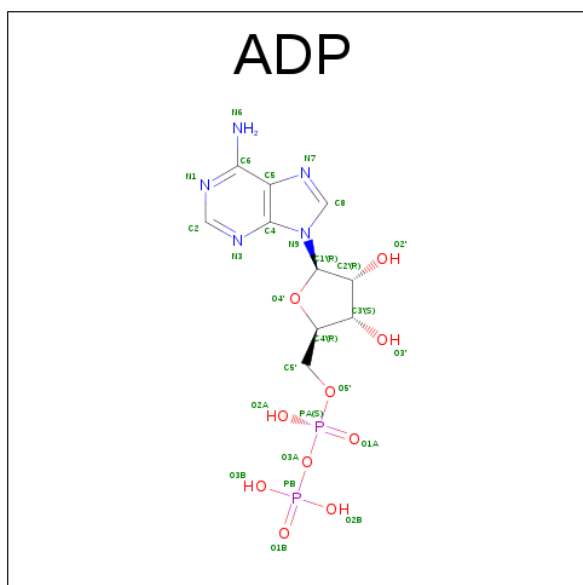
- Molecule 1 is a protein called ABC transporter homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	578	Total	C	N	O	S	1	0	0
			4584	2967	774	834	9			
1	B	578	Total	C	N	O	S	1	0	0
			4584	2967	774	834	9			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

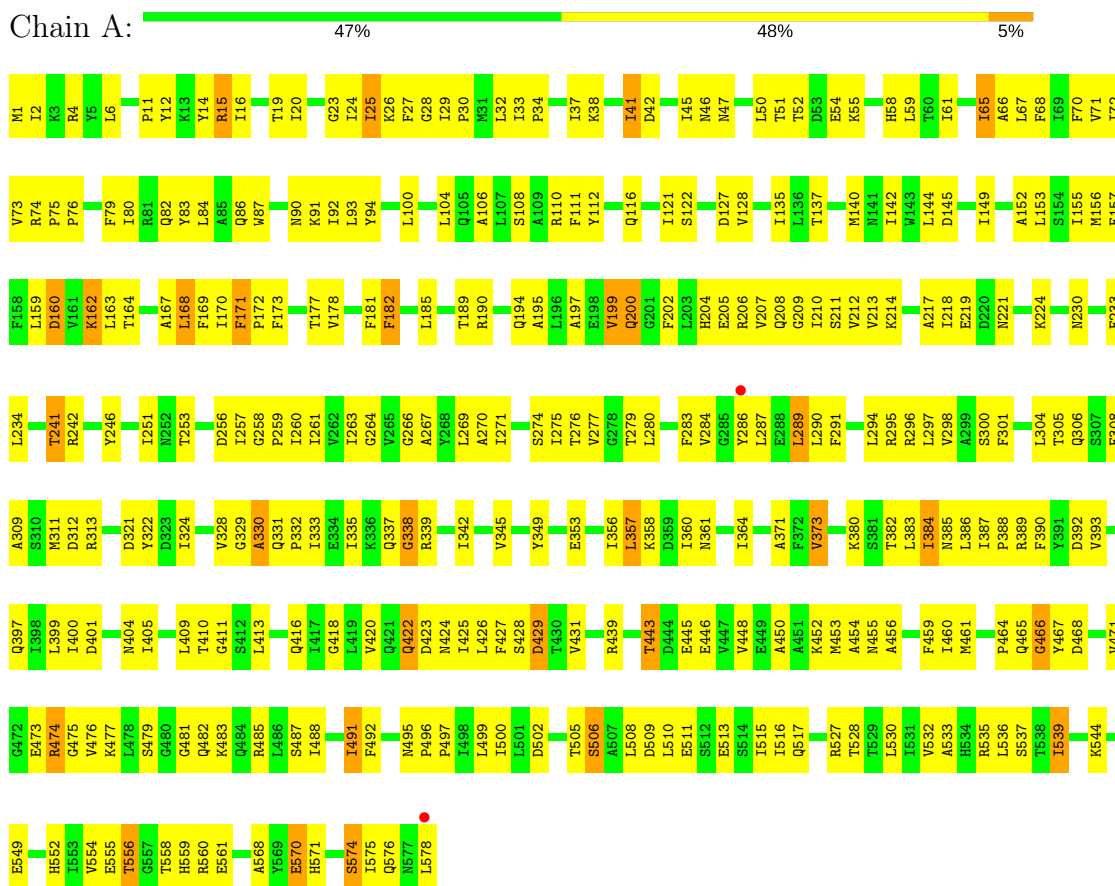
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O	0	0
			8	8		
4	B	8	Total	O	0	0
			8	8		

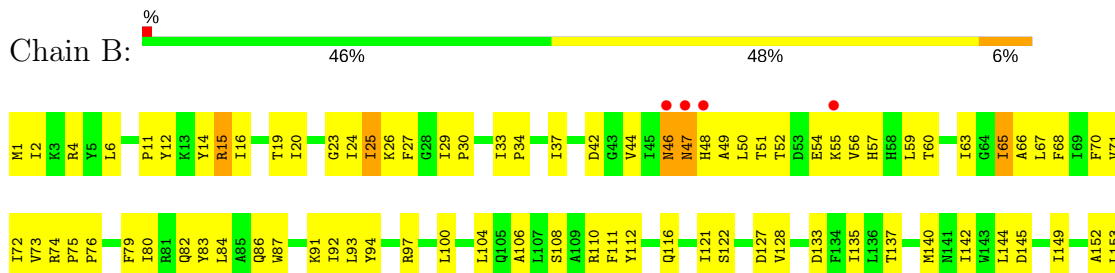
### 3 Residue-property plots

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



#### • Molecule 1: ABC transporter homolog



S154	F233	T305	Y391	G466	I539
I155	L234	Q306	D392	Y467	K544
M156	F308	S307	V393	D468	E549
L159	T241	A309	Q397	V471	H552
D160	R242	S310	I398	G472	I553
V161	Y246	K311	L399	E473	V554
K162	I251	D312	I400	R474	E555
L163	T252	R313	D401	G475	V556
T164	T253	I321	N404	V476	G557
L165	D256	Y322	I405	K477	L478
A166	I257	S323	L409	S479	S479
A167	G258	I324	T410	G480	H559
L168	G259	V328	G411	G481	R560
F169	P259	G329	S412	Q482	E561
I170	I260	A330	L413	K483	A568
F171	I261	Q331	R414	Q484	Y569
P172	V262	P332	R415	R485	E570
F173	I263	I333	Q416	T488	H571
T177	G264	E334	I417	I491	S574
V178	V265	I335	G418	F492	I575
F181	G266	K336	L419	P495	Q576
F182	A267	Q337	V420	L496	N577
L185	Y268	G338	Q421	P497	L578
L189	L269	R339	Q422	L498	
R190	A270	I342	D423	I499	
	I271	V345	N424	L500	
	G273	Y349	I425	L501	
Q194	S274	E353	L426	D502	
A195	I275	I356	F427	T505	
L196	T276	L357	S428	S506	
A197	V277	K358	D429	A507	
E198	G278	D359	V431	L508	
V199	T279	K360	R439	D509	
Q200	L280	N361	T443	L510	
G201	F283	I364	D444	E511	
L203	V284	V373	E445	S512	
H204	G285	A371	E446	E513	
E205	Y286	V373	V447	S514	
R206	L287	K380	V448	L515	
V207	E288	S381	E449	L516	
Q208	L289	T382	A450	D517	
G209	L290	L383	A451	R527	
I210	F291	I384	K452	T528	
S211	L294	N385	M453	T529	
V212	R295	L386	A454	L530	
V213	L297	I387	A456	V532	
K214	V298	P388	F459	L531	
	A217	R389	I460	A533	
A217	E299	F390	M461	H534	
I218	S300		P464	R535	
E219	F301		Q465	L536	
I220	T302			S537	
N221	I303			T538	
K224	L304				

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.28Å 103.95Å 181.01Å 90.00° 97.99° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00 29.88 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00) 99.2 (29.88-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.83 (at 3.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.255 , 0.272 (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
Wilson B-factor (Å <sup>2</sup> )	78.1	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 74.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9240	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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: NA, ADP

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	0.41	0/4669	0.66	1/6328 (0.0%)
1	B	0.52	3/4669 (0.1%)	0.68	3/6328 (0.0%)
All	All	0.47	3/9338 (0.0%)	0.67	4/12656 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	47	ASN	CB-CG	15.97	1.87	1.51
1	B	46	ASN	C-N	-9.51	1.12	1.34
1	B	48	HIS	CA-CB	8.89	1.73	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	49	ALA	CB-CA-C	5.39	118.18	110.10
1	A	357	LEU	N-CA-C	-5.15	97.09	111.00
1	B	46	ASN	O-C-N	5.12	130.89	122.70
1	B	357	LEU	N-CA-C	-5.01	97.47	111.00

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	4584	0	4713	346	0
1	B	4584	0	4712	373	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	7	0
3	B	27	0	12	5	0
4	A	8	0	0	3	0
4	B	8	0	0	2	0
All	All	9240	0	9449	658	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 35.

The worst 5 of 658 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:47:ASN:CG	1:B:47:ASN:CB	1.87	1.42
1:A:15:ARG:H	1:A:15:ARG:HD2	1.01	1.15
1:B:15:ARG:H	1:B:15:ARG:HD2	1.01	1.09
1:A:52:THR:HA	1:A:55:LYS:HE2	1.10	1.09
1:B:44:VAL:HG13	1:B:55:LYS:HB2	1.36	1.08

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	576/578 (100%)	487 (84%)	73 (13%)	16 (3%)	6	29
1	B	576/578 (100%)	480 (83%)	80 (14%)	16 (3%)	6	29
All	All	1152/1156 (100%)	967 (84%)	153 (13%)	32 (3%)	6	29

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	ILE
1	A	41	ILE
1	A	338	GLY
1	B	25	ILE
1	B	338	GLY

### 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	499/499 (100%)	474 (95%)	25 (5%)	28	67
1	B	499/499 (100%)	473 (95%)	26 (5%)	27	65
All	All	998/998 (100%)	947 (95%)	51 (5%)	28	66

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	556	THR
1	B	159	LEU
1	B	539	ILE
1	B	15	ARG
1	B	162	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	455	ASN
1	A	465	GLN
1	B	200	GLN
1	A	397	GLN
1	B	306	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z  > 2$
3	ADP	A	700	-	25,29,29	1.18	2 (8%)	24,45,45	2.00	3 (12%)
3	ADP	B	701	-	25,29,29	1.15	2 (8%)	24,45,45	2.04	3 (12%)

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
3	ADP	A	700	-	-	0/12/32/32	0/3/3/3
3	ADP	B	701	-	-	0/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	701	ADP	C8-N7	-2.53	1.29	1.34
3	A	700	ADP	C8-N7	-2.51	1.30	1.34
3	B	701	ADP	O4'-C1'	3.43	1.46	1.41
3	A	700	ADP	O4'-C1'	3.67	1.46	1.41

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	ADP	N3-C2-N1	-8.30	121.63	128.86
3	A	700	ADP	N3-C2-N1	-8.11	121.80	128.86
3	B	701	ADP	C4-C5-N7	-2.25	107.23	109.41
3	A	700	ADP	C4-C5-N7	-2.13	107.35	109.41
3	B	701	ADP	C2'-C3'-C4'	2.33	107.15	102.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	700	ADP	7	0
3	B	701	ADP	5	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 [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, 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	578/578 (100%)	-0.52	2 (0%) 93 82	56, 97, 162, 200	2 (0%)
1	B	578/578 (100%)	-0.48	4 (0%) 87 67	54, 95, 162, 200	2 (0%)
All	All	1156/1156 (100%)	-0.50	6 (0%) 90 74	54, 96, 162, 200	4 (0%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	47	ASN	5.9
1	B	46	ASN	4.5
1	B	48	HIS	3.0
1	A	286	TYR	2.7
1	A	578	LEU	2.6

### 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( $\text{\AA}^2$ )	Q<0.9
2	NA	B	910	1/1	0.90	0.28	2.46	31,31,31,31	0
2	NA	A	900	1/1	0.96	0.23	0.93	24,24,24,24	0
3	ADP	B	701	27/27	0.91	0.20	0.47	78,83,84,85	0
3	ADP	A	700	27/27	0.91	0.19	0.35	80,83,85,85	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.