



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 09:04 PM GMT

PDB ID : 3CF3  
Title : Structure of P97/vcp in complex with ADP  
Authors : Davies, J.M.; Delabarre, B.; Brunger, A.T.; Weis, W.I.  
Deposited on : 2008-03-01  
Resolution : 4.25 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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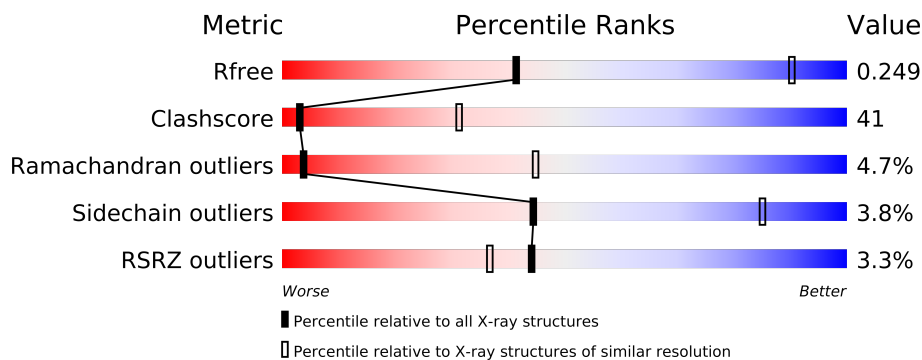
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	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 4.25 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	1013 (5.02-3.50)
Clashscore	79885	1277 (5.02-3.50)
Ramachandran outliers	78287	1208 (5.02-3.50)
Sidechain outliers	78261	1190 (5.02-3.50)
RSRZ outliers	66119	1013 (5.02-3.50)

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	806	
1	B	806	
1	C	806	

## 2 Entry composition i

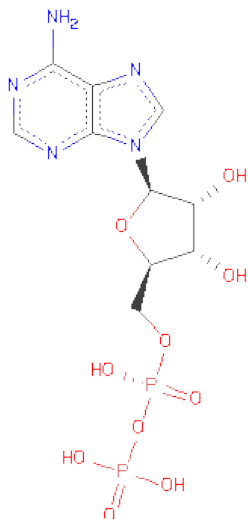
There are 2 unique types of molecules in this entry. The entry contains 17139 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	723	Total	C	N	O	S	0	0	0
			5659	3561	996	1072	30			
1	B	723	Total	C	N	O	S	0	0	0
			5659	3561	996	1072	30			
1	C	723	Total	C	N	O	S	0	0	0
			5659	3561	996	1072	30			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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

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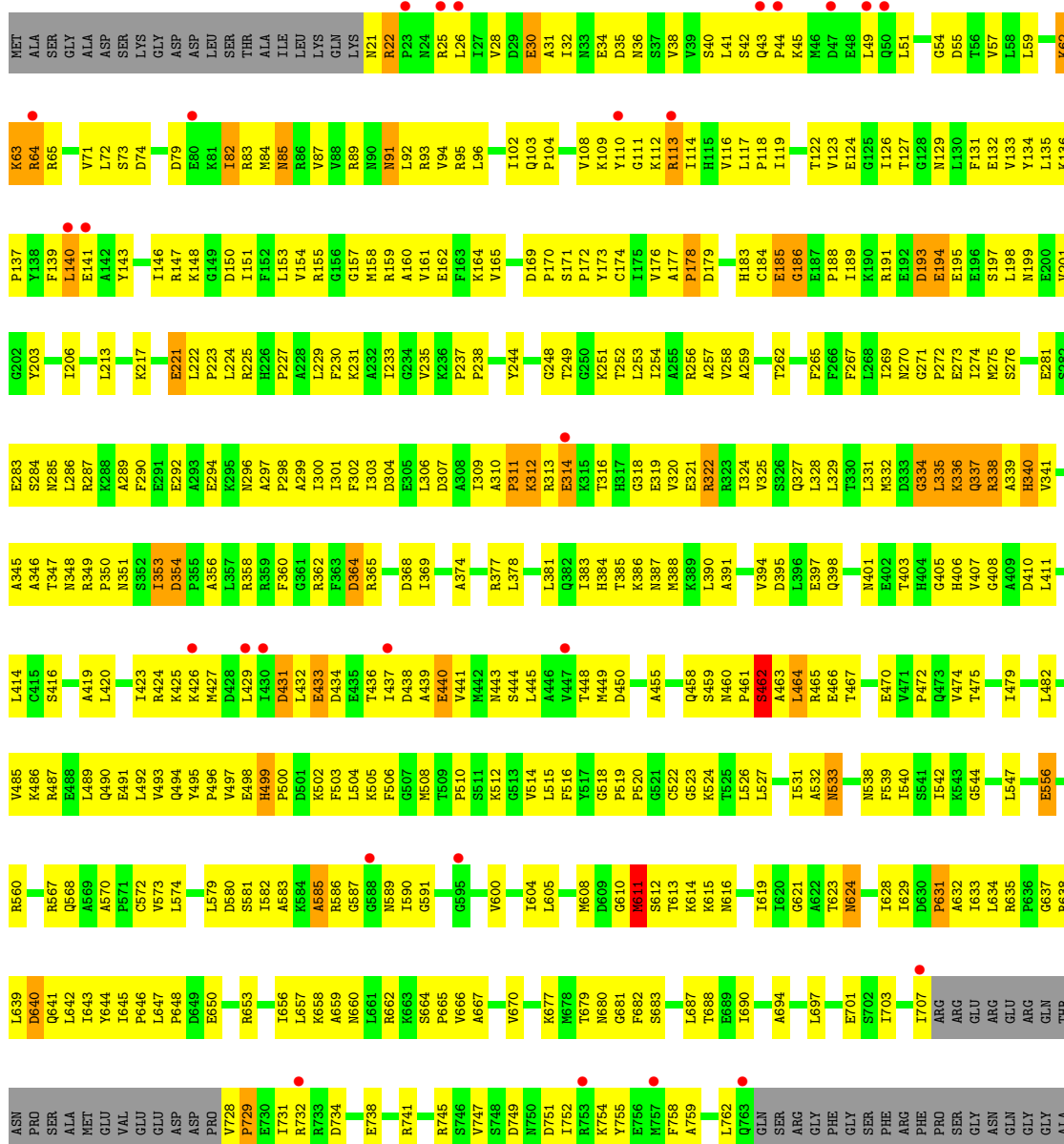
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

### 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: Transitional endoplasmic reticulum ATPase

Chain A: 



Chain B:



GLY	ALA	ARG	GLN	GLU	D640	Q568	L492	L420	N348	S284	T206	F139	V71
GLY	GLY	GLY	GLY	GLY	L642	A569	Q494	T423	R349	N285	L213	L140	L72
PRO	PRO	THR	THR	THR	L643	P571	Y495	R424	P350	L286		L141	S73
ASN	ASN	ASN	ASN	ASN	L644	C572	P496	K425		R287	K217	A142	D74
GLN	GLN	PRO	PRO	PRO	L645	V573	V497	K426	D354	A289		Y143	
GLY	GLY	SER	SER	SER	F646	L574	E498	K427	P355	F290	E221	T146	D75
SER	SER	ALA	ALA	ALA	L647	F575	H499	D428	A356	E291	L222		
MET	MET	GLY	GLY	GLY	F648	F576	P500	L429	R357	A292	L223	R147	D79
GLY	GLY	GLU	GLU	GLU	D649	D577	D501	L430	R358	A293	L224	K148	K81
GLY	GLY	VAL	VAL	VAL	E650	E578	K502	D431	R359	E294		D150	I82
THR	THR	GLU	GLU	GLU	R653	L579	F503	L432	F360	K295	P227	I151	R83
GLY	GLY	GLU	GLU	GLU		D580	L504	E433	G361	N296	A228	F152	M84
GLY	GLY	ASP	ASP	ASP		S581	K505		R362	A297	L229	L153	R86
SER	SER	ASP	ASP	ASP	L656	L582		E435	F363	A299	K231	Y154	V87
VAL	VAL	PRO	PRO	PRO	L657		M508	T436	D364	A299			
TYR	TYR	W728	W728	TYR	K658	R586	T509	L437	R365	I300	A232	G157	V88
THR	THR	P729	P729	THR	A659	G587	P510	D438	G368	I301	I233	M158	R89
GLU	GLU	E730	E730	GLU	R660	G588	S511	A439	F302	I302	G234	R159	R90
ASP	ASP	I731	I731	ASP	L661	N589	K512	E440	L369	I303	G236	A160	N91
ASN	ASN	R732	R732	ASN	R662	I590	G513	V441		D304	K236	V161	R92
ASP	ASP	R733	R733	ASP	K663	G591	V514	M442	A374		P237	E162	R93
ASP	ASP	D734	D734	ASP	P664	D592	L515			I309	P238	F163	V94
ASP	ASP			ASP	S665	G593	F516	S444	R377	A310		K164	R95
LEU	LEU	P666	P666	LEU	V666	G594	G517	L445	L378	P311	Y244	V165	L96
LEU	LEU	A667	A667	LEU									
TYR	TYR	E738	E738	TYR		V600	G518	M449	L381	R313	G248	D169	I102
GLY	GLY	R741	R741	GLY	V670		P519	P520	Q382	R315	G249	P170	Q103
		R745	R745			I604	G521	A455	K315	K315	G250	S171	P104
		S746	S746		K677	L605	C522		H384	T316	K251	P172	
		V747	V747		P678		G523	Q458	K386	H317	T252	K173	
		S748	S748		T679	M608	K524	S459	K386	G318	L253	C174	V108
		D749	D749		N680	D609	L525	N460	N387	E319	T254	I175	K109
		N750	N750		G610	G510	L526	P461	M388	V320		V176	G111
		D751	D751		F682	N611	L527	S462	K389	E321	A257	A177	Y110
		I752	I752		S683	S612		A463	L390		V258	P178	K112
					G684	T613	I531	L464	A391	R322	A259	D179	R113
		Y755	Y755			K614	A532						I114
		E756	E756			K615	N633	R485	V394	I324	N260	H183	H115
		M757	M757		T688	N616							

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	163.97Å 178.93Å 320.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 4.25 29.94 – 4.25	Depositor EDS
% Data completeness (in resolution range)	86.4 (40.00-4.25) 92.9 (29.94-4.25)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 4.26Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.198 , 0.226 0.225 , 0.249	Depositor DCC
$R_{free}$ test set	2301 reflections (7.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	143.2	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 154.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 63665 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	17139	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	205.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.92% 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: 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	0.38	0/5751	0.87	9/7767 (0.1%)
1	B	0.37	0/5751	0.87	9/7767 (0.1%)
1	C	0.38	0/5751	0.88	9/7767 (0.1%)
All	All	0.38	0/17253	0.87	27/23301 (0.1%)

There are no bond length outliers.

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	322	ARG	NE-CZ-NH2	-29.67	105.46	120.30
1	A	338	ARG	NE-CZ-NH1	-29.13	105.74	120.30
1	B	287	ARG	NE-CZ-NH2	-28.38	106.11	120.30
1	A	338	ARG	NE-CZ-NH2	27.38	133.99	120.30
1	B	287	ARG	NE-CZ-NH1	27.28	133.94	120.30

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	5659	0	5731	495	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5659	0	5731	491	0
1	C	5659	0	5731	466	0
2	A	54	0	24	6	0
2	B	54	0	24	4	0
2	C	54	0	24	3	0
All	All	17139	0	17265	1421	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 41.

The worst 5 of 1421 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:206:ILE:CD1	1:A:213:LEU:HD11	1.25	1.64
1:B:206:ILE:CD1	1:B:213:LEU:HD11	1.24	1.61
1:C:206:ILE:CD1	1:C:213:LEU:HD11	1.25	1.59
1:A:206:ILE:HD11	1:A:213:LEU:CD1	1.55	1.34
1:C:206:ILE:HD11	1:C:213:LEU:CD1	1.55	1.34

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	719/806 (89%)	566 (79%)	119 (17%)	34 (5%)	4	45
1	B	719/806 (89%)	564 (78%)	123 (17%)	32 (4%)	4	46
1	C	719/806 (89%)	561 (78%)	122 (17%)	36 (5%)	3	43
All	All	2157/2418 (89%)	1691 (78%)	364 (17%)	102 (5%)	4	45

5 of 102 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	LYS

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Mol	Chain	Res	Type
1	A	85	ASN
1	A	140	LEU
1	A	185	GLU
1	A	312	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	615/678 (91%)	590 (96%)	25 (4%)	41	83
1	B	615/678 (91%)	593 (96%)	22 (4%)	47	86
1	C	615/678 (91%)	592 (96%)	23 (4%)	45	86
All	All	1845/2034 (91%)	1775 (96%)	70 (4%)	44	85

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	287	ARG
1	B	440	GLU
1	C	579	LEU
1	B	314	GLU
1	B	340	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	285	ASN
1	B	348	ASN
1	C	616	ASN
1	B	327	GLN
1	B	401	ASN

### 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 ⓘ

6 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	ADP	A	807	-	29,29,29	1.83	9 (31%)	45,45,45	2.64	9 (20%)
2	ADP	A	900	-	29,29,29	1.68	7 (24%)	45,45,45	2.47	4 (8%)
2	ADP	B	807	-	29,29,29	1.64	5 (17%)	45,45,45	2.47	7 (15%)
2	ADP	B	900	-	29,29,29	1.50	4 (13%)	45,45,45	2.28	7 (15%)
2	ADP	C	807	-	29,29,29	1.99	5 (17%)	45,45,45	2.45	7 (15%)
2	ADP	C	900	-	29,29,29	1.70	6 (20%)	45,45,45	2.46	6 (13%)

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	ADP	A	807	-	-	0/16/32/32	0/1/3/3
2	ADP	A	900	-	-	0/16/32/32	0/1/3/3
2	ADP	B	807	-	-	0/16/32/32	0/1/3/3
2	ADP	B	900	-	-	0/16/32/32	0/1/3/3
2	ADP	C	807	-	-	0/16/32/32	0/1/3/3
2	ADP	C	900	-	-	0/16/32/32	0/1/3/3

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	807	ADP	C4-N9	-6.90	1.27	1.37
2	A	900	ADP	O4'-C1'	3.99	1.47	1.41
2	A	807	ADP	PA-O3A	-3.91	1.52	1.59
2	C	900	ADP	O4'-C1'	3.90	1.47	1.41
2	B	900	ADP	C4-N9	-3.78	1.32	1.37

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	807	ADP	N3-C2-N1	-14.13	116.89	128.71
2	C	900	ADP	N3-C2-N1	-13.74	117.22	128.71
2	A	900	ADP	N3-C2-N1	-13.59	117.35	128.71
2	B	807	ADP	N3-C2-N1	-13.47	117.45	128.71
2	C	807	ADP	N3-C2-N1	-13.46	117.45	128.71

There are no chirality outliers.

There are no torsion outliers.

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	723/806 (89%)	0.20	27 (3%) 39 33	40, 202, 284, 353	0
1	B	723/806 (89%)	0.15	19 (2%) 53 42	39, 200, 282, 352	0
1	C	723/806 (89%)	0.20	26 (3%) 41 34	38, 202, 283, 352	0
All	All	2169/2418 (89%)	0.18	72 (3%) 44 37	38, 201, 283, 353	0

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	435	GLU	5.9
1	C	757	MET	4.5
1	B	109	LYS	3.9
1	C	190	LYS	3.7
1	A	23	PRO	3.7

### 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( $\text{\AA}^2$ )	Q<0.9
2	ADP	B	900	27/27	0.25	1.07	106,157,202,277	0
2	ADP	C	807	27/27	0.32	1.02	144,177,268,273	0
2	ADP	A	900	27/27	0.23	0.50	122,174,209,218	0
2	ADP	A	807	27/27	0.26	0.41	133,149,222,335	0
2	ADP	C	900	27/27	0.26	0.07	118,157,187,206	0
2	ADP	B	807	27/27	0.22	-0.08	139,163,218,268	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.