



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2018 – 12:44 PM EST

PDB ID : 5WAG
Title : ADC-7 in complex with boronic acid transition state inhibitor S06017
Authors : Powers, R.A.; Wallar, B.J.
Deposited on : 2017-06-26
Resolution : 1.93 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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 : rb-20030736
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) : rb-20030736

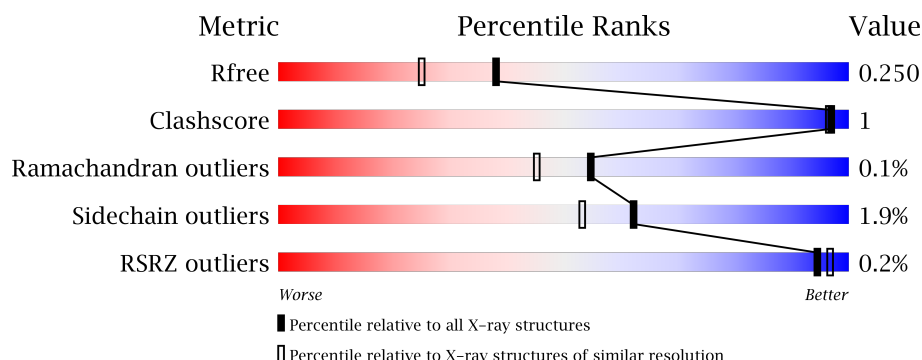
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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	3233 (1.96-1.92)
Clashscore	112137	3430 (1.96-1.92)
Ramachandran outliers	110173	3395 (1.96-1.92)
Sidechain outliers	110143	3395 (1.96-1.92)
RSRZ outliers	101464	3250 (1.96-1.92)

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 ≥ 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	361	<div> <div>94%</div> <div>5% .</div> </div>
1	B	361	<div> <div>96%</div> <div>. .</div> </div>
1	C	361	<div> <div>93%</div> <div>5% .</div> </div>
1	D	361	<div> <div>93%</div> <div>6% .</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	A0V	A	401	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11516 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.

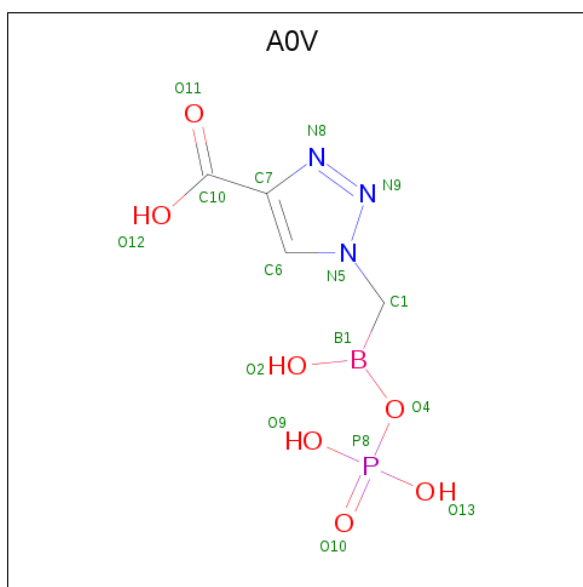
- Molecule 1 is a protein called Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	358	Total	C	N	O	S	0	3	0
			2820	1815	467	529	9			
1	A	355	Total	C	N	O	S	0	0	0
			2769	1781	460	519	9			
1	C	355	Total	C	N	O	S	0	0	0
			2729	1760	451	509	9			
1	D	356	Total	C	N	O	S	0	1	0
			2730	1758	452	511	9			

There are 4 discrepancies between the modelled and reference sequences:

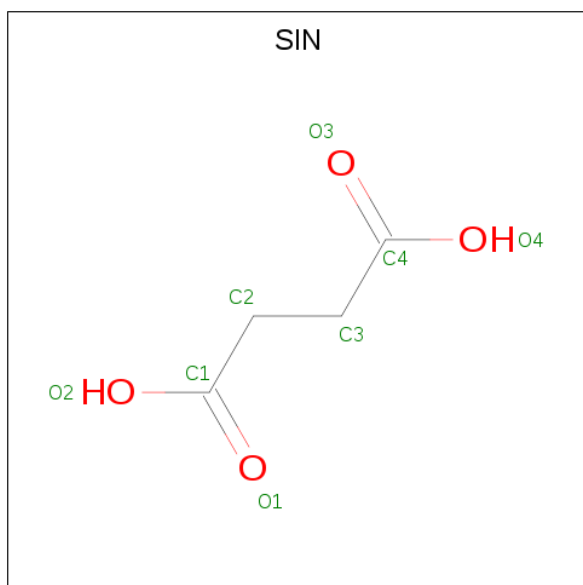
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	MET	-	expression tag	UNP Q6DRA1
A	-1	MET	-	expression tag	UNP Q6DRA1
C	-1	MET	-	expression tag	UNP Q6DRA1
D	-1	MET	-	expression tag	UNP Q6DRA1

- Molecule 2 is 1-{{hydroxy(phosphonooxy)boranyl}methyl}-1H-1,2,3-triazole-4-carboxylic acid (three-letter code: A0V) (formula: C₄H₇BN₃O₇P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	B	C	N	O	P		
2	B	1	Total 16	1	4	3	7	1	0	0
2	A	1	Total 16	1	4	3	7	1	0	0
2	C	1	Total 16	1	4	3	7	1	0	0
2	D	1	Total 16	1	4	3	7	1	0	0

- Molecule 3 is SUCCINIC ACID (three-letter code: SIN) (formula: C₄H₆O₄).

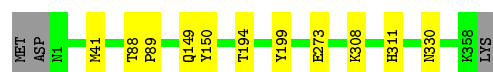


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	4	4		

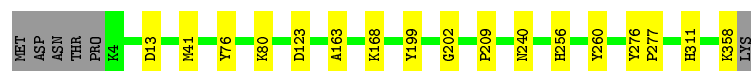
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	168	Total	O	0	2
			170	170		
4	A	114	Total	O	0	2
			116	116		
4	C	45	Total	O	0	2
			47	47		
4	D	62	Total	O	0	1
			63	63		

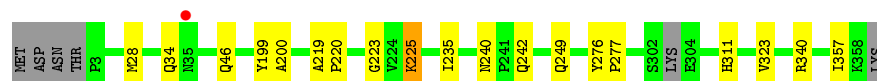
- Molecule 1: Beta-lactamase



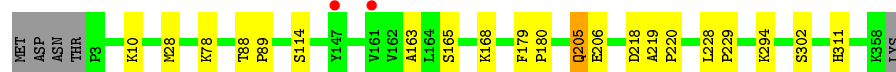
- Molecule 1: Beta-lactamase



- Molecule 1: Beta-lactamase



- Molecule 1: Beta-lactamase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.67Å 80.90Å 105.34Å 90.00° 113.36° 90.00°	Depositor
Resolution (Å)	81.40 – 1.93 81.40 – 1.93	Depositor EDS
% Data completeness (in resolution range)	97.3 (81.40-1.93) 97.4 (81.40-1.93)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.186 , 0.247 0.195 , 0.250	Depositor DCC
R_{free} test set	4987 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11516	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.98 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.3641e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A0V, SIN

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	0.89	1/2836 (0.0%)	0.87	1/3859 (0.0%)
1	B	0.92	0/2898	0.88	0/3940
1	C	0.75	0/2796	0.79	2/3809 (0.1%)
1	D	0.79	0/2801	0.84	2/3820 (0.1%)
All	All	0.84	1/11331 (0.0%)	0.85	5/15428 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	260	TYR	CE1-CZ	-5.16	1.31	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	218	ASP	CB-CG-OD1	8.21	125.69	118.30
1	A	13	ASP	CB-CG-OD1	5.89	123.60	118.30
1	D	28	MET	CG-SD-CE	5.78	109.45	100.20
1	C	340	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	C	28	MET	CG-SD-CE	5.17	108.47	100.20

There are no chirality outliers.

There are no planarity outliers.

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	2769	0	2721	7	0
1	B	2820	0	2795	3	0
1	C	2729	0	2644	8	0
1	D	2730	0	2630	7	0
2	A	16	0	0	0	0
2	B	16	0	0	1	0
2	C	16	0	0	0	0
2	D	16	0	0	0	0
3	A	8	0	4	2	0
4	A	116	0	0	0	0
4	B	170	0	0	0	0
4	C	47	0	0	0	0
4	D	63	0	0	1	0
All	All	11516	0	10794	25	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 1.

All (25) 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:256:HIS:ND1	3:A:402:SIN:H22	2.03	0.73
1:C:235:ILE:HD11	1:C:323:VAL:HG13	1.76	0.68
1:A:358:LYS:HE2	1:A:358:LYS:HA	1.95	0.49
1:C:219:ALA:HB3	1:C:220:PRO:HD3	1.94	0.48
1:C:235:ILE:HD11	1:C:323:VAL:CG1	2.45	0.47
1:D:205:GLN:HG3	4:D:551:HOH:O	2.13	0.47
1:C:242:GLN:HA	1:C:249:GLN:NE2	2.31	0.46
1:A:163:ALA:HB1	1:A:168:LYS:O	2.15	0.45
1:A:276:TYR:CD1	1:A:277:PRO:HA	2.51	0.45
1:D:163:ALA:HB1	1:D:168:LYS:O	2.16	0.44
1:C:276:TYR:CD1	1:C:277:PRO:HA	2.53	0.44
1:D:88:THR:HB	1:D:89:PRO:HD2	1.98	0.44
1:C:223:GLY:O	1:C:225:LYS:CE	2.66	0.44
1:A:202:GLY:O	1:A:209:PRO:HA	2.18	0.43
1:D:228:LEU:HB3	1:D:229:PRO:HD3	2.01	0.43
1:D:205:GLN:HE21	1:D:206:GLU:HG2	1.83	0.43
1:C:46:GLN:HG3	1:C:200:ALA:HA	2.01	0.42
1:D:219:ALA:HB3	1:D:220:PRO:HD3	2.00	0.42
1:A:256:HIS:ND1	3:A:402:SIN:C2	2.79	0.41
1:B:273:GLU:OE2	1:B:308:LYS:HG2	2.21	0.41
1:B:88:THR:HB	1:B:89:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:GLN:NE2	1:C:357:ILE:CG2	2.83	0.41
1:A:76:TYR:CZ	1:A:80:LYS:HE2	2.57	0.40
1:D:179:PHE:HB2	1:D:180:PRO:HD3	2.03	0.40
1:B:150:TYR:OH	2:B:401:A0V:O13	2.29	0.40

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	353/361 (98%)	337 (96%)	16 (4%)	0	100	100
1	B	359/361 (99%)	351 (98%)	8 (2%)	0	100	100
1	C	351/361 (97%)	338 (96%)	13 (4%)	0	100	100
1	D	355/361 (98%)	344 (97%)	10 (3%)	1 (0%)	44	33
All	All	1418/1444 (98%)	1370 (97%)	47 (3%)	1 (0%)	55	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	114	SER

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	298/319 (93%)	293 (98%)	5 (2%)	66	58
1	B	308/319 (97%)	302 (98%)	6 (2%)	62	53
1	C	286/319 (90%)	282 (99%)	4 (1%)	71	65
1	D	285/319 (89%)	278 (98%)	7 (2%)	53	41
All	All	1177/1276 (92%)	1155 (98%)	22 (2%)	62	53

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	41	MET
1	B	149	GLN
1	B	194	THR
1	B	199	TYR
1	B	311	HIS
1	B	330	ASN
1	A	41	MET
1	A	123	ASP
1	A	199	TYR
1	A	240	ASN
1	A	311	HIS
1	C	199	TYR
1	C	225	LYS
1	C	240	ASN
1	C	311	HIS
1	D	10	LYS
1	D	78	LYS
1	D	165	SER
1	D	205	GLN
1	D	294	LYS
1	D	302	SER
1	D	311	HIS

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

Mol	Chain	Res	Type
1	B	35	ASN
1	A	36	ASN
1	A	240	ASN
1	A	330	ASN
1	C	34	GLN

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Mol	Chain	Res	Type
1	C	236	HIS
1	C	240	ASN
1	D	205	GLN

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](#)

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	A0V	A	401	1	10,16,16	1.81	4 (40%)	8,23,23	2.12	1 (12%)
3	SIN	A	402	-	1,7,7	0.12	0	2,8,8	1.96	1 (50%)
2	A0V	B	401	1	10,16,16	2.13	4 (40%)	8,23,23	1.76	1 (12%)
2	A0V	C	401	1	10,16,16	1.94	3 (30%)	8,23,23	2.81	5 (62%)
2	A0V	D	401	1	10,16,16	1.82	3 (30%)	8,23,23	2.45	3 (37%)

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	A0V	A	401	1	-	0/0/13/13	0/1/1/1
3	SIN	A	402	-	-	0/1/5/5	0/0/0/0
2	A0V	B	401	1	-	0/0/13/13	0/1/1/1
2	A0V	C	401	1	-	0/0/13/13	0/1/1/1
2	A0V	D	401	1	-	0/0/13/13	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	A0V	C6-N5	-2.82	1.32	1.35
2	A	401	A0V	C6-N5	-2.57	1.32	1.35
2	C	401	A0V	C6-C7	2.01	1.39	1.37
2	A	401	A0V	N8-N9	2.16	1.37	1.34
2	D	401	A0V	N9-N5	2.29	1.38	1.34
2	D	401	A0V	N8-N9	2.46	1.37	1.34
2	A	401	A0V	C6-C7	2.53	1.40	1.37
2	B	401	A0V	N9-N5	2.70	1.39	1.34
2	B	401	A0V	B1-C1	2.92	1.60	1.56
2	B	401	A0V	C6-C7	3.01	1.40	1.37
2	A	401	A0V	B1-C1	3.01	1.60	1.56
2	D	401	A0V	C6-C7	3.42	1.41	1.37
2	C	401	A0V	N8-N9	3.82	1.39	1.34
2	B	401	A0V	N8-N9	3.98	1.39	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	A0V	O13-P8-O4	-3.75	97.55	109.52
2	C	401	A0V	O9-P8-O4	-3.40	98.65	109.52
2	D	401	A0V	O13-P8-O4	-2.91	100.23	109.52
3	A	402	SIN	C2-C3-C4	-2.58	108.26	112.66
2	C	401	A0V	O13-P8-O10	2.10	118.72	110.50
2	C	401	A0V	O9-P8-O13	2.48	117.62	107.61
2	D	401	A0V	O9-P8-O13	2.61	118.15	107.61
2	B	401	A0V	N8-N9-N5	4.12	110.42	107.31
2	C	401	A0V	N8-N9-N5	4.91	111.01	107.31
2	A	401	A0V	N8-N9-N5	5.44	111.42	107.31
2	D	401	A0V	N8-N9-N5	5.50	111.46	107.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	SIN	2	0
2	B	401	A0V	1	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, 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	355/361 (98%)	-0.43	0	100 100	22, 32, 47, 77	0
1	B	358/361 (99%)	-0.49	0	100 100	20, 28, 41, 52	0
1	C	355/361 (98%)	-0.18	1 (0%)	93 96	29, 43, 61, 82	0
1	D	356/361 (98%)	-0.16	2 (0%)	89 92	21, 42, 64, 83	0
All	All	1424/1444 (98%)	-0.32	3 (0%)	94 97	20, 36, 58, 83	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	147	TYR	3.3
1	D	161	VAL	2.1
1	C	35	ASN	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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	A0V	A	401	16/16	0.96	0.12	2.54	33,43,52,54	0
2	A0V	B	401	16/16	0.97	0.10	1.60	29,43,56,58	0
3	SIN	A	402	8/8	0.78	0.15	1.45	55,58,66,72	0
2	A0V	C	401	16/16	0.98	0.10	0.54	35,45,58,63	0
2	A0V	D	401	16/16	0.93	0.11	0.11	34,47,54,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.