



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 08:11 AM EDT

PDB ID : 5J4N  
Title : Crystal structure of the L-arginine/agmatine antiporter AdiC in complex with agmatine at 2.6 Angstrom resolution  
Authors : Jeckelmann, J.M.; Ilgue, H.; Fotiadis, D.  
Deposited on : 2016-04-01  
Resolution : 2.59 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.37.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

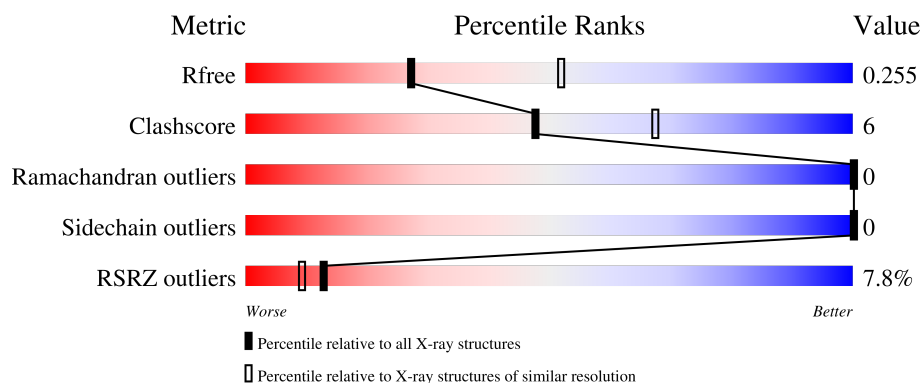
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	453	<div> <div>7%</div> <div>85%</div> <div>12%</div> <div>.</div> </div>
1	B	453	<div> <div>8%</div> <div>85%</div> <div>11%</div> <div>.</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6533 atoms, of which 28 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.

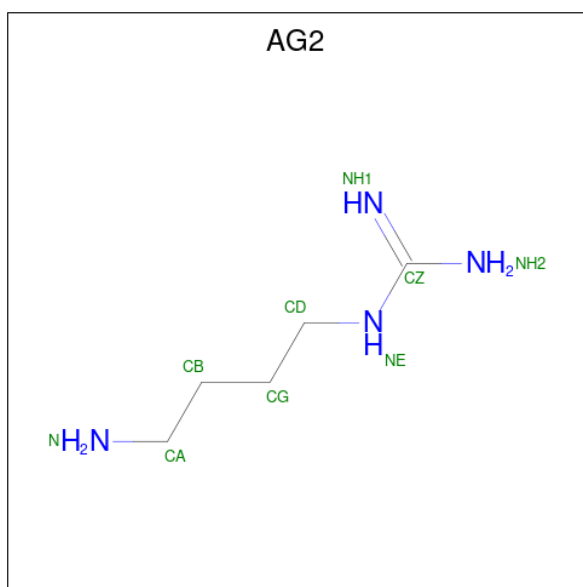
- Molecule 1 is a protein called Arginine/agmatine antiporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3240	2149	518	551	22			
1	B	436	Total	C	N	O	S	0	0	0
			3235	2146	517	550	22			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	446	LEU	-	expression tag	UNP P60063
A	447	GLU	-	expression tag	UNP P60063
A	448	LEU	-	expression tag	UNP P60063
A	449	GLU	-	expression tag	UNP P60063
A	450	VAL	-	expression tag	UNP P60063
A	451	LEU	-	expression tag	UNP P60063
A	452	PHE	-	expression tag	UNP P60063
A	453	GLN	-	expression tag	UNP P60063
B	446	LEU	-	expression tag	UNP P60063
B	447	GLU	-	expression tag	UNP P60063
B	448	LEU	-	expression tag	UNP P60063
B	449	GLU	-	expression tag	UNP P60063
B	450	VAL	-	expression tag	UNP P60063
B	451	LEU	-	expression tag	UNP P60063
B	452	PHE	-	expression tag	UNP P60063
B	453	GLN	-	expression tag	UNP P60063

- Molecule 2 is AGMATINE (three-letter code: AG2) (formula: C<sub>5</sub>H<sub>14</sub>N<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	N	0	0
			23	5	14	4		
2	B	1	Total	C	H	N	0	0
			23	5	14	4		

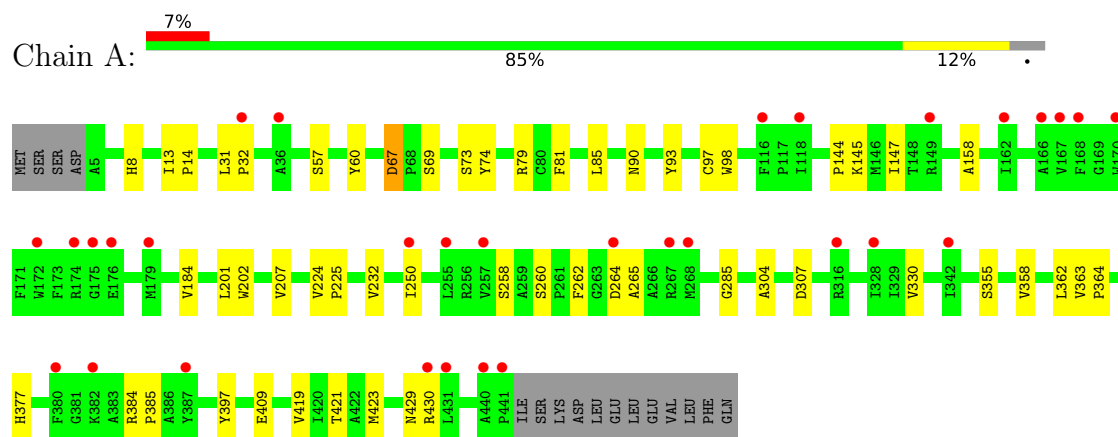
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	2	Total	O	0	0
			2	2		

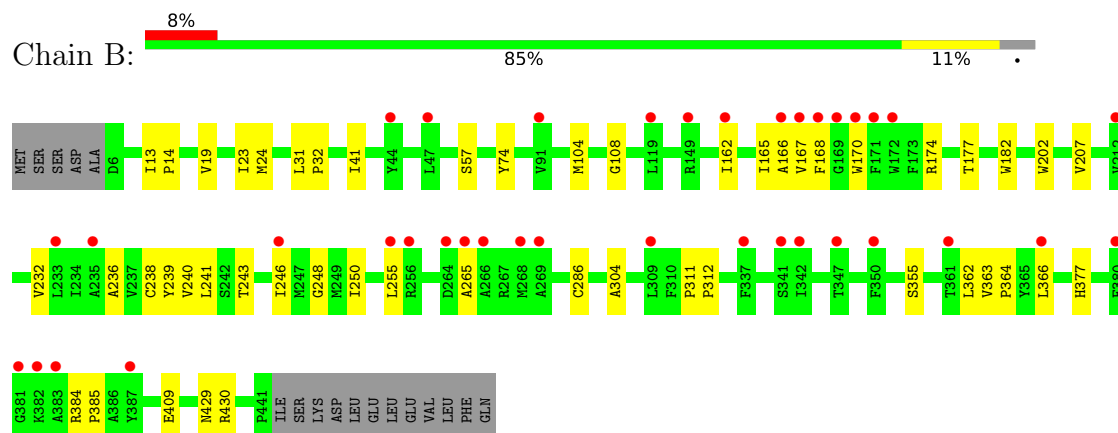
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Arginine/agmatine antiporter



#### • Molecule 1: Arginine/agmatine antiporter



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.77Å 175.63Å 72.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.44 – 2.59 49.44 – 2.59	Depositor EDS
% Data completeness (in resolution range)	98.0 (49.44-2.59) 98.5 (49.44-2.59)	Depositor EDS
$R_{merge}$	0.01	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.91 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.221 , 0.251 0.227 , 0.255	Depositor DCC
$R_{free}$ test set	2092 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.2	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 59.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6533	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AG2

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	0/3326	0.46	1/4553 (0.0%)
1	B	0.47	1/3321 (0.0%)	0.48	0/4546
All	All	0.42	1/6647 (0.0%)	0.47	1/9099 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	239	TYR	CE1-CZ	-5.14	1.31	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	ASP	C-N-CD	5.18	139.27	128.40

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	3240	0	3355	47	0
1	B	3235	0	3350	44	0
2	A	9	14	13	0	0
2	B	9	14	13	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	10	0	0	3	0
3	B	2	0	0	0	0
All	All	6505	28	6731	81	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 6.

All (81) 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:421:THR:HG21	1:B:366:LEU:CD2	1.80	1.12
1:B:429:ASN:O	1:B:430:ARG:HG2	1.48	1.11
1:A:421:THR:HG21	1:B:366:LEU:HD21	1.31	1.11
1:A:429:ASN:O	1:A:430:ARG:HG2	1.52	1.08
1:A:421:THR:CG2	1:B:366:LEU:HD21	1.89	1.03
1:A:250:ILE:HD11	1:A:265:ALA:HB2	1.47	0.97
1:A:258:SER:OG	1:A:264:ASP:OD2	1.87	0.92
1:B:429:ASN:O	1:B:430:ARG:CG	2.19	0.90
1:A:429:ASN:O	1:A:430:ARG:CG	2.18	0.90
1:B:166:ALA:O	1:B:170:TRP:CD1	2.25	0.90
1:A:250:ILE:HD11	1:A:265:ALA:CB	2.03	0.88
1:A:69:SER:O	3:A:601:HOH:O	1.97	0.80
1:A:250:ILE:CD1	1:A:265:ALA:HB2	2.13	0.78
1:A:307:ASP:OD2	3:A:602:HOH:O	2.06	0.73
1:B:174:ARG:O	1:B:177:THR:OG1	2.11	0.66
1:A:184:VAL:HG12	1:A:184:VAL:O	2.00	0.61
1:A:260:SER:O	1:A:264:ASP:N	2.31	0.61
1:B:19:VAL:O	1:B:23:ILE:HG13	2.00	0.60
1:A:67:ASP:OD2	1:A:79:ARG:NE	2.32	0.59
1:B:32:PRO:HB3	1:B:246:ILE:HG21	1.84	0.59
1:B:177:THR:OG1	1:B:248:GLY:O	2.21	0.59
1:A:421:THR:CG2	1:B:366:LEU:CD2	2.62	0.58
1:B:108:GLY:CA	1:B:286:CYS:SG	2.92	0.57
1:A:13:ILE:HB	1:A:14:PRO:HD3	1.87	0.57
1:B:13:ILE:HB	1:B:14:PRO:HD3	1.86	0.56
1:B:167:VAL:HG12	1:B:168:PHE:CD1	2.40	0.56
1:A:421:THR:CB	1:B:366:LEU:HD21	2.36	0.55
1:B:250:ILE:HD11	1:B:265:ALA:CB	2.36	0.55
1:B:104:MET:O	1:B:286:CYS:SG	2.64	0.55
1:A:201:LEU:O	1:A:397:TYR:OH	2.19	0.54
1:A:250:ILE:HD11	1:A:265:ALA:HB1	1.88	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ILE:HG21	1:B:238:CYS:HB3	1.89	0.54
1:A:144:PRO:HA	1:A:147:ILE:HG22	1.89	0.53
1:B:41:ILE:HG13	1:B:182:TRP:CZ2	2.44	0.53
1:B:355:SER:HB3	1:B:409:GLU:HG2	1.92	0.52
1:B:108:GLY:HA3	1:B:286:CYS:SG	2.50	0.51
1:A:98:TRP:CB	1:A:330:VAL:HG13	2.40	0.51
1:B:24:MET:HE3	1:B:238:CYS:HB2	1.92	0.50
1:A:377:HIS:CG	1:B:430:ARG:HB3	2.46	0.50
1:B:162:ILE:O	1:B:165:ILE:HG22	2.12	0.50
1:A:363:VAL:HB	1:A:364:PRO:HD3	1.94	0.48
1:A:430:ARG:HB3	1:B:377:HIS:CG	2.49	0.48
1:A:429:ASN:C	1:A:430:ARG:HG2	2.27	0.48
1:B:250:ILE:HD11	1:B:265:ALA:HB2	1.95	0.47
1:A:421:THR:HG21	1:B:366:LEU:HD23	1.85	0.47
1:A:74:TYR:CZ	1:A:304:ALA:HA	2.50	0.47
1:A:8:HIS:HA	1:A:145:LYS:HD2	1.97	0.46
1:A:98:TRP:HB3	1:A:330:VAL:HG13	1.98	0.46
1:A:202:TRP:CH2	1:A:362:LEU:HD11	2.51	0.46
1:B:429:ASN:C	1:B:430:ARG:HG2	2.27	0.45
1:B:363:VAL:HB	1:B:364:PRO:HD3	1.98	0.45
1:A:57:SER:HB3	1:A:232:VAL:HG21	1.97	0.45
1:A:60:TYR:OH	1:A:73:SER:OG	2.30	0.45
1:A:384:ARG:CZ	1:B:430:ARG:CZ	2.95	0.45
1:B:207:VAL:HG23	1:B:232:VAL:HG21	1.98	0.45
1:A:419:VAL:O	1:A:423:MET:HG3	2.17	0.44
1:B:243:THR:O	1:B:246:ILE:HG22	2.17	0.44
1:A:384:ARG:N	1:A:385:PRO:HD2	2.33	0.44
1:B:57:SER:HB3	1:B:232:VAL:HG21	1.99	0.43
1:B:236:ALA:O	1:B:240:VAL:HG23	2.17	0.43
1:A:158:ALA:HB2	1:A:285:GLY:HA3	2.00	0.43
1:B:207:VAL:HG23	1:B:232:VAL:CG2	2.48	0.42
1:A:224:VAL:HB	1:A:225:PRO:HD3	2.01	0.42
1:B:250:ILE:HD11	1:B:265:ALA:HB1	2.00	0.42
1:B:246:ILE:HG12	1:B:255:LEU:HD11	2.02	0.42
1:A:430:ARG:CZ	1:B:384:ARG:CZ	2.97	0.42
1:B:384:ARG:N	1:B:385:PRO:HD2	2.34	0.42
1:A:81:PHE:HB3	1:A:85:LEU:HD12	2.02	0.42
1:B:31:LEU:N	1:B:32:PRO:HD2	2.35	0.42
1:A:32:PRO:HG3	1:A:262:PHE:CE1	2.55	0.41
1:B:74:TYR:CZ	1:B:304:ALA:HA	2.55	0.41
1:A:202:TRP:CZ3	1:A:358:VAL:HG12	2.55	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:ALA:HB1	1:B:241:LEU:HD13	2.03	0.41
1:A:207:VAL:HG23	1:A:232:VAL:HG21	2.02	0.41
1:B:311:PRO:HA	1:B:312:PRO:HD3	1.94	0.41
1:A:90:ASN:HB3	3:A:603:HOH:O	2.21	0.41
1:A:93:TYR:CE2	1:A:97:CYS:SG	3.14	0.41
1:A:31:LEU:N	1:A:32:PRO:HD2	2.36	0.40
1:B:202:TRP:CH2	1:B:362:LEU:HD11	2.56	0.40
1:A:355:SER:OG	1:A:409:GLU:HG3	2.21	0.40
1:A:429:ASN:C	1:A:430:ARG:CG	2.88	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	435/453 (96%)	431 (99%)	4 (1%)	0	100	100
1	B	434/453 (96%)	430 (99%)	4 (1%)	0	100	100
All	All	869/906 (96%)	861 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	335/351 (95%)	335 (100%)	0	100	100
1	B	335/351 (95%)	335 (100%)	0	100	100
All	All	670/702 (95%)	670 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes 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 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

2 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	AG2	A	501	-	8,8,8	2.26	2 (25%)	7,8,8	0.79	0
2	AG2	B	501	-	8,8,8	2.33	2 (25%)	7,8,8	0.68	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	AG2	A	501	-	-	0/6/6/6	-
2	AG2	B	501	-	-	0/6/6/6	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	AG2	CZ-NE	5.56	1.44	1.33
2	A	501	AG2	CZ-NE	5.37	1.43	1.33
2	A	501	AG2	CZ-NH2	2.86	1.46	1.34
2	B	501	AG2	CZ-NH2	2.85	1.46	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	437/453 (96%)	0.67	31 (7%) 16 11	49, 62, 96, 115	0
1	B	436/453 (96%)	0.73	37 (8%) 10 7	48, 66, 104, 130	0
All	All	873/906 (96%)	0.70	68 (7%) 13 9	48, 64, 100, 130	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	166	ALA	6.4
1	B	168	PHE	5.3
1	A	170	TRP	5.0
1	B	170	TRP	4.7
1	A	441	PRO	4.5
1	A	440	ALA	4.3
1	B	268	MET	4.3
1	A	32	PRO	4.2
1	A	268	MET	4.1
1	B	162	ILE	4.0
1	B	342	ILE	3.9
1	A	250	ILE	3.7
1	B	266	ALA	3.4
1	B	264	ASP	3.4
1	A	387	TYR	3.3
1	B	383	ALA	3.2
1	A	257	VAL	3.2
1	B	269	ALA	3.2
1	B	382	LYS	3.2
1	A	176	GLU	3.1
1	B	381	GLY	3.1
1	A	168	PHE	3.0
1	B	255	LEU	3.0
1	A	175	GLY	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	172	TRP	3.0
1	A	179	MET	2.9
1	A	264	ASP	2.9
1	A	267	ARG	2.8
1	A	431	LEU	2.8
1	A	430	ARG	2.8
1	A	255	LEU	2.8
1	B	341	SER	2.8
1	B	387	TYR	2.7
1	B	167	VAL	2.7
1	B	166	ALA	2.7
1	A	380	PHE	2.7
1	A	149	ARG	2.7
1	A	116	PHE	2.7
1	A	162	ILE	2.7
1	B	235	ALA	2.6
1	A	328	ILE	2.6
1	B	350	PHE	2.6
1	B	347	THR	2.6
1	B	169	GLY	2.6
1	B	47	LEU	2.5
1	B	171	PHE	2.5
1	A	174	ARG	2.5
1	B	366	LEU	2.4
1	B	256	ARG	2.3
1	A	316	ARG	2.3
1	B	265	ALA	2.3
1	B	119	LEU	2.3
1	B	246	ILE	2.2
1	B	172	TRP	2.2
1	A	167	VAL	2.2
1	A	36	ALA	2.2
1	B	212	VAL	2.2
1	A	342	ILE	2.2
1	B	233	LEU	2.1
1	B	44	TYR	2.1
1	B	361	THR	2.1
1	A	382	LYS	2.1
1	B	149	ARG	2.1
1	B	91	VAL	2.1
1	B	337	PHE	2.1
1	A	118	ILE	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	309	LEU	2.0
1	B	380	PHE	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 monosaccharides 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	AG2	B	501	9/9	0.92	0.34	49,62,69,75	0
2	AG2	A	501	9/9	0.98	0.22	42,53,63,67	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.