



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:45 AM UTC

PDB ID : 5J4N / pdb_00005j4n
Title : Crystal structure of the L-arginine/agmatine antiporter AdiC in complex with agmatine at 2.6 Angstroem 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

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

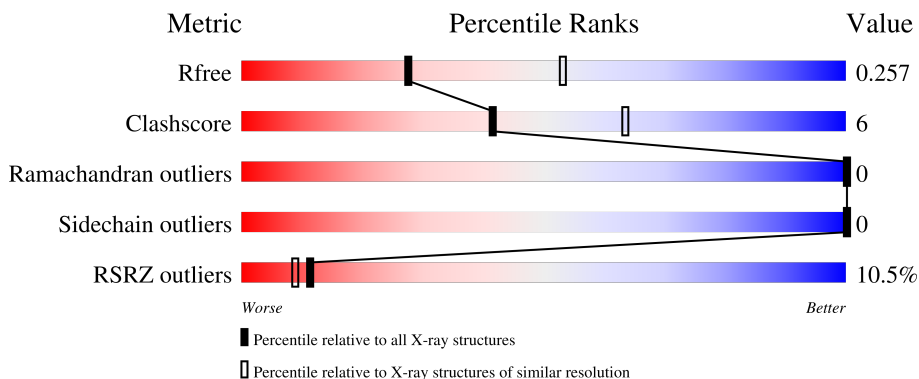
1 Overall quality at a glance

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 ≥ 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	10% 84% 12% .
1	B	453	10% 84% 12% .

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.

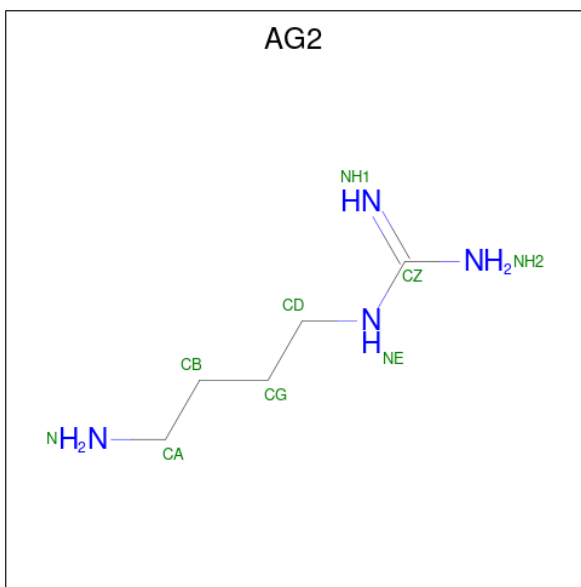
- Molecule 1 is a protein called Arginine/agmatine antiporter.

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 (CCD ID: AG2) (formula: C₅H₁₄N₄).



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		

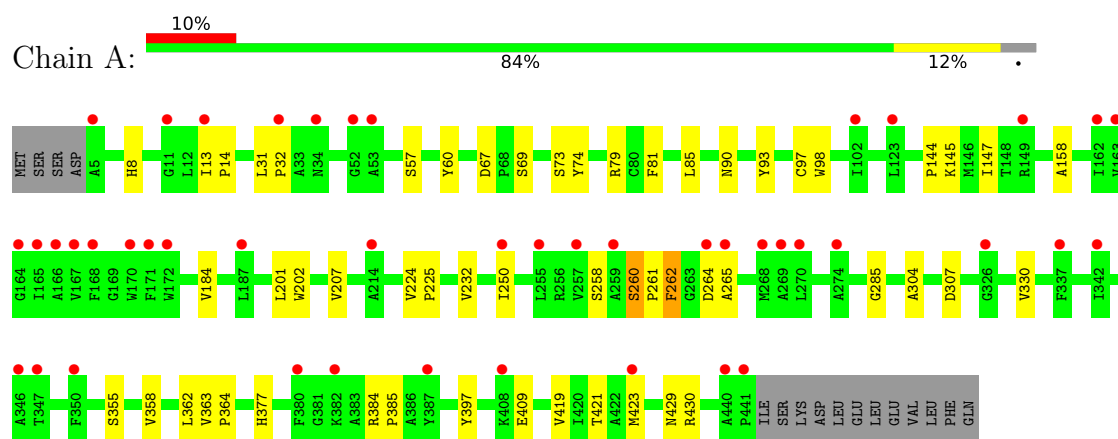
- Molecule 3 is water.

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

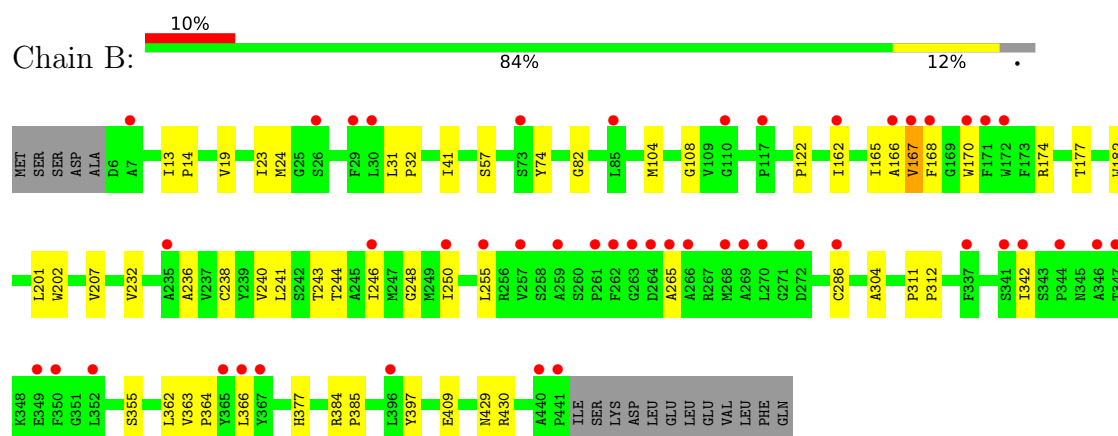
3 Residue-property plots

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, α , β , γ	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) 98.4 (49.44-2.59)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.91 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.221 , 0.251 0.230 , 0.257	Depositor DCC
R_{free} test set	2092 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	62.2	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.49	0/3326	0.79	4/4553 (0.1%)
1	B	0.61	0/3321	0.81	3/4546 (0.1%)
All	All	0.55	0/6647	0.80	7/9099 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	167	VAL	N-CA-C	7.63	117.70	110.53
1	A	262	PHE	N-CA-C	-6.22	104.50	111.28
1	A	260	SER	CA-C-N	5.89	125.59	119.05
1	A	260	SER	C-N-CA	5.89	125.59	119.05
1	B	82	GLY	CA-C-N	5.68	125.36	119.05
1	B	82	GLY	C-N-CA	5.68	125.36	119.05
1	A	261	PRO	N-CA-C	5.06	120.56	113.53

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	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	9	14	13	0	0
2	B	9	14	13	0	0
3	A	10	0	0	3	0
3	B	2	0	0	0	0
All	All	6505	28	6731	84	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 (84) 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:A:429:ASN:C	1:A:430:ARG:HG2	2.27	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:B:429:ASN:C	1:B:430:ARG:HG2	2.27	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:VAL:O	1:B:244:THR:OG1	2.15	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
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: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:60:TYR:OH	1:A:73:SER:OG	2.30	0.49
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: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: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:384:ARG:CZ	1:B:430:ARG:CZ	2.95	0.45
1:A:429:ASN:C	1:A:430:ARG:CG	2.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:PRO:HB2	1:B:342:ILE:C	2.45	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
1:B:201:LEU:O	1:B:397:TYR:OH	2.30	0.41
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:24:MET:HE3	1:B:238:CYS:HB2	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

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	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

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. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	B	198	ASN
1	B	252	ASN

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 oligosaccharides 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	B	501	-	8,8,8	2.45	2 (25%)	7,8,8	0.69	0
2	AG2	A	501	-	8,8,8	2.39	2 (25%)	7,8,8	0.80	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	B	501	-	-	0/6/6/6	-
2	AG2	A	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	5.70	1.44	1.33
2	A	501	AG2	CZ-NE	5.50	1.43	1.33
2	A	501	AG2	CZ-NH2	3.34	1.46	1.34
2	B	501	AG2	CZ-NH2	3.33	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, 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	437/453 (96%)	0.73	45 (10%)	12 9	49, 62, 96, 115	0
1	B	436/453 (96%)	0.79	47 (10%)	11 8	48, 66, 104, 130	0
All	All	873/906 (96%)	0.76	92 (10%)	11 9	48, 64, 100, 130	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	168	PHE	5.0
1	B	342	ILE	4.8
1	A	5	ALA	4.7
1	A	270	LEU	4.7
1	A	268	MET	4.6
1	B	265	ALA	4.6
1	B	259	ALA	4.5
1	B	268	MET	4.3
1	B	162	ILE	4.2
1	A	32	PRO	4.2
1	B	26	SER	4.1
1	B	166	ALA	4.1
1	B	269	ALA	4.0
1	A	166	ALA	3.9
1	A	259	ALA	3.9
1	A	441	PRO	3.7
1	B	171	PHE	3.7
1	B	167	VAL	3.7
1	B	366	LEU	3.6
1	A	171	PHE	3.6
1	B	7	ALA	3.5
1	B	286	CYS	3.5
1	A	342	ILE	3.5
1	B	350	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	235	ALA	3.2
1	A	149	ARG	3.2
1	A	346	ALA	3.1
1	A	250	ILE	3.1
1	B	341	SER	3.1
1	A	387	TYR	3.0
1	B	352	LEU	3.0
1	B	264	ASP	3.0
1	A	347	THR	3.0
1	A	162	ILE	3.0
1	B	29	PHE	2.9
1	B	270	LEU	2.9
1	B	73	SER	2.8
1	A	264	ASP	2.8
1	B	272	ASP	2.8
1	A	11	GLY	2.7
1	A	53	ALA	2.7
1	B	440	ALA	2.7
1	A	269	ALA	2.7
1	A	163	VAL	2.7
1	B	266	ALA	2.7
1	A	172	TRP	2.7
1	B	347	THR	2.7
1	A	102	ILE	2.6
1	B	441	PRO	2.6
1	B	346	ALA	2.6
1	B	255	LEU	2.6
1	B	261	PRO	2.6
1	A	168	PHE	2.6
1	B	337	PHE	2.6
1	A	440	ALA	2.5
1	A	52	GLY	2.5
1	A	408	LYS	2.4
1	A	337	PHE	2.4
1	A	423	MET	2.4
1	B	263	GLY	2.4
1	A	13	ILE	2.4
1	A	165	ILE	2.4
1	A	350	PHE	2.4
1	A	167	VAL	2.4
1	A	170	TRP	2.4
1	A	164	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	326	GLY	2.3
1	B	257	VAL	2.3
1	B	246	ILE	2.3
1	A	187	LEU	2.3
1	B	367	TYR	2.3
1	B	170	TRP	2.2
1	A	257	VAL	2.2
1	B	344	PRO	2.2
1	A	274	ALA	2.2
1	B	30	LEU	2.2
1	B	250	ILE	2.2
1	A	380	PHE	2.2
1	A	382	LYS	2.2
1	B	396	LEU	2.1
1	A	255	LEU	2.1
1	B	172	TRP	2.1
1	A	34	ASN	2.1
1	B	110	GLY	2.1
1	B	349	GLU	2.1
1	B	365	TYR	2.1
1	A	214	ALA	2.1
1	B	262	PHE	2.0
1	A	265	ALA	2.0
1	A	123	LEU	2.0
1	B	117	PRO	2.0
1	B	85	LEU	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 oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
2	AG2	B	501	9/9	0.91	0.34	49,62,69,75	0
2	AG2	A	501	9/9	0.94	0.18	42,53,63,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.