



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:17 AM GMT

PDB ID : 2CJA
Title : CRYSTAL STRUCTURE OF METHANOSARCINA BARKERI SERYL-
TRNA SYNTHETASE COMPLEXED WITH ATP
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Deposited on : 2006-03-30
Resolution : 2.20 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

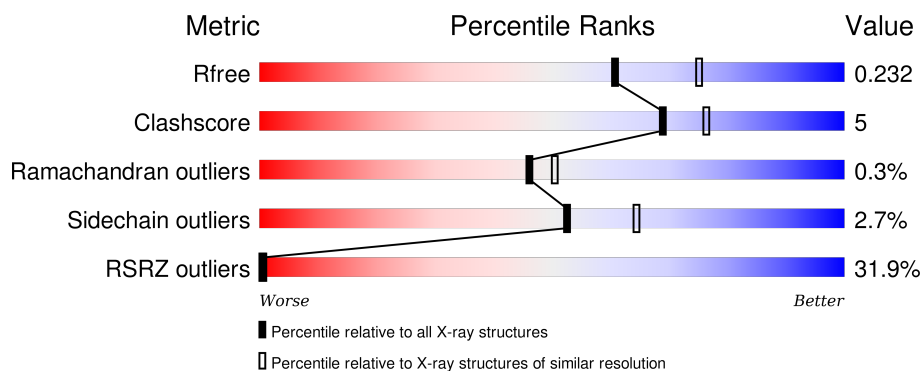
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	522	<div> <div>33%</div> <div>79%</div> <div>11%</div> <div>9%</div> </div>
1	B	522	<div> <div>25%</div> <div>81%</div> <div>12%</div> <div>6%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8418 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 SERYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	Se	0	2	0
			3916	2517	674	705	6	14			
1	B	489	Total	C	N	O	S	Se	0	1	0
			3982	2555	682	725	6	14			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Mg	0	0
			2	2		

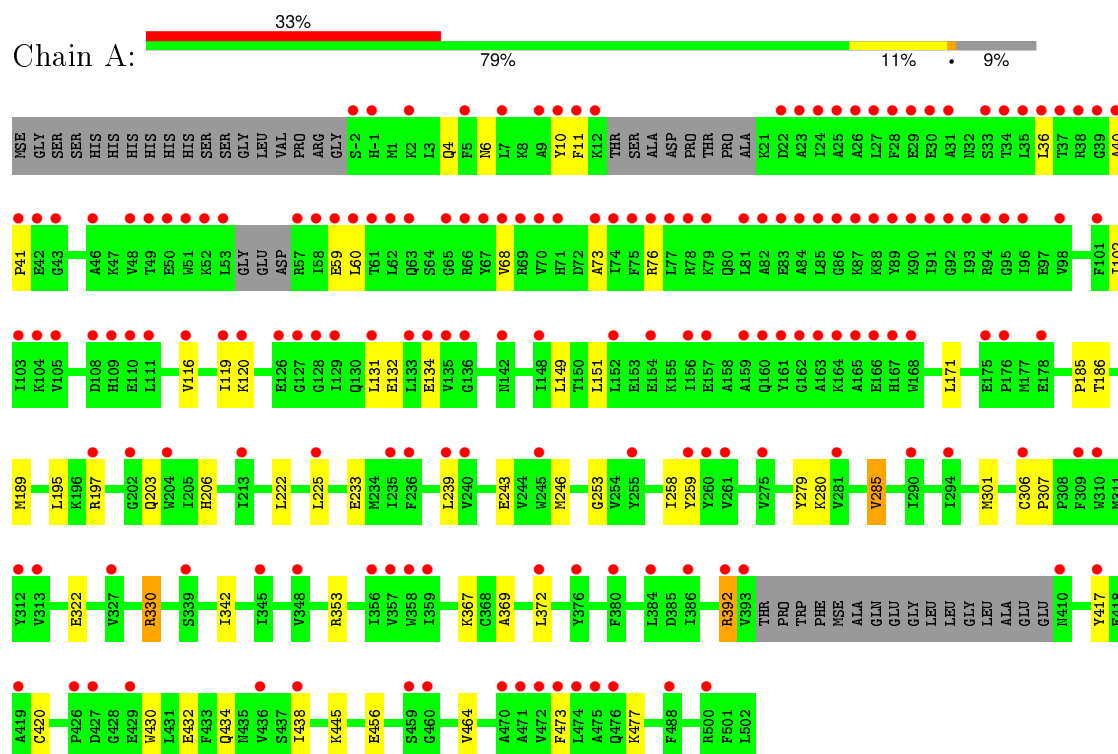
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	221	Total	O	0	0
			221	221		
6	B	231	Total	O	0	0
			231	231		

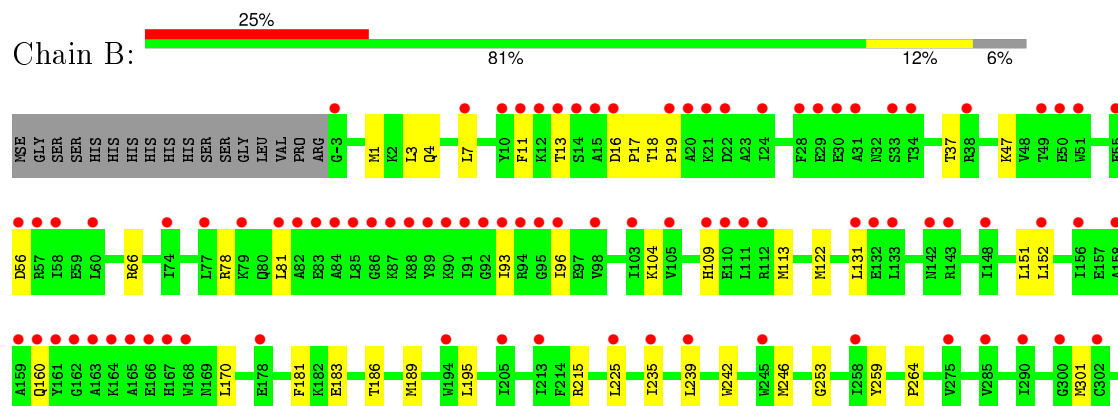
3 Residue-property plots

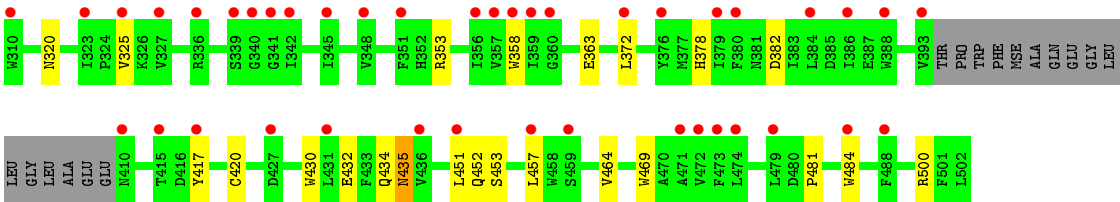
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: SERYL-TRNA SYNTHETASE



• Molecule 1: SERYL-TRNA SYNTHETASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	97.31Å 97.31Å 270.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.74 – 2.20 19.74 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.74-2.20) 99.1 (19.74-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.203 , 0.233 0.204 , 0.232	Depositor DCC
R_{free} test set	3781 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 57.8	EDS
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 75456 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8418	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, ZN, ATP, CL

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	0.39	0/4005	0.52	0/5385
1	B	0.39	0/4075	0.53	0/5487
All	All	0.39	0/8080	0.52	0/10872

There are no bond length outliers.

There are no bond angle outliers.

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	3916	0	3870	37	0
1	B	3982	0	3923	43	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	31	0	12	0	0
4	B	31	0	12	0	0
5	B	2	0	0	0	0
6	A	221	0	0	2	0
6	B	231	0	0	1	0
All	All	8418	0	7817	73	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 5.

All (73) 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:259:TYR:HB3	1:A:301[B]:MSE:HE2	1.48	0.94
1:B:186:THR:HA	1:B:189:MSE:HE2	1.54	0.89
1:B:186:THR:HA	1:B:189:MSE:CE	2.04	0.87
1:B:259:TYR:HB3	1:B:301[B]:MSE:HE2	1.59	0.84
1:A:186:THR:HA	1:A:189:MSE:HE3	1.69	0.75
1:A:259:TYR:CB	1:A:301[B]:MSE:HE2	2.21	0.70
1:A:243:GLU:HA	1:A:246:MSE:HE3	1.73	0.70
1:A:301[B]:MSE:HE1	1:B:239:LEU:HD12	1.74	0.69
1:A:186:THR:HA	1:A:189:MSE:CE	2.23	0.67
1:B:4:GLN:HG3	1:B:104:LYS:HB2	1.78	0.65
1:B:259:TYR:CB	1:B:301[B]:MSE:CE	2.74	0.65
1:B:417:TYR:HB2	1:B:434:GLN:HB3	1.79	0.64
1:B:186:THR:CA	1:B:189:MSE:HE2	2.29	0.61
1:B:18:THR:N	1:B:19:PRO:HD2	2.16	0.61
1:B:259:TYR:CB	1:B:301[B]:MSE:HE2	2.31	0.61
1:A:197[B]:ARG:HH12	1:A:203:GLN:H	1.49	0.60
1:A:417:TYR:HB2	1:A:434:GLN:HB3	1.83	0.60
1:A:102:ILE:HG12	1:A:132:GLU:HG3	1.87	0.57
1:A:171:LEU:HD11	1:A:392:ARG:HG3	1.87	0.56
1:A:259:TYR:CB	1:A:301[B]:MSE:CE	2.82	0.56
1:A:280:LYS:HD2	1:B:151:LEU:HD13	1.88	0.56
1:B:259:TYR:HB3	1:B:301[B]:MSE:CE	2.29	0.55
1:A:68:VAL:HG12	6:A:2016:HOH:O	2.06	0.55
1:B:1:MSE:HE3	6:B:2005:HOH:O	2.07	0.55
1:A:369:ALA:HB2	1:A:438:ILE:HD11	1.88	0.55
1:B:13:THR:HG21	1:B:17:PRO:HG3	1.89	0.55
1:A:259:TYR:HB3	1:A:301[B]:MSE:CE	2.30	0.54
1:A:206:HIS:HB2	1:B:235:ILE:HB	1.90	0.54
1:B:11:PHE:CD1	1:B:93:ILE:HD11	2.43	0.53
1:B:259:TYR:CB	1:B:301[B]:MSE:HE3	2.38	0.53
1:A:11:PHE:HE2	1:A:60:LEU:HD11	1.73	0.53
1:B:320:ASN:HD21	1:B:453:SER:H	1.57	0.52
1:A:258:ILE:O	1:B:264:PRO:HD3	2.10	0.52
1:B:259:TYR:HB2	1:B:301[B]:MSE:HE3	1.92	0.52
1:B:122:MSE:HG3	1:B:131:LEU:HD23	1.92	0.51
1:B:81:LEU:HD22	1:B:93:ILE:HD12	1.92	0.51
1:B:181:PHE:CZ	1:B:183:GLU:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:THR:HA	1:B:189:MSE:HE3	1.90	0.50
1:A:445:LYS:NZ	1:A:456:GLU:OE1	2.45	0.49
1:B:131:LEU:HD11	1:B:152:LEU:HD22	1.95	0.48
1:A:4:GLN:HE21	1:A:6:ASN:HD21	1.60	0.48
1:B:451:LEU:HB2	1:B:457:LEU:HG	1.95	0.48
1:A:233:GLU:OE2	1:A:330:ARG:HD2	2.14	0.48
1:A:120:LYS:HB2	1:A:134:GLU:HG3	1.96	0.47
1:B:78:ARG:HD2	1:B:96:ILE:HD11	1.97	0.46
1:A:116:VAL:HB	1:A:119:ILE:HD12	1.97	0.46
1:A:306:CYS:SG	1:A:307:PRO:HD3	2.56	0.46
1:B:320:ASN:HD22	1:B:452:GLN:HB3	1.81	0.46
1:B:3:LEU:HD23	1:B:66:ARG:HB3	1.98	0.46
1:A:36:LEU:HD23	1:A:76:ARG:HD2	1.97	0.45
1:A:285:VAL:HG11	1:B:242:TRP:HB3	1.97	0.45
1:A:185:PRO:O	1:A:189:MSE:HG3	2.17	0.45
1:A:11:PHE:CE2	1:A:60:LEU:HD11	2.52	0.45
1:A:40:ALA:HA	1:A:41:PRO:HD3	1.87	0.45
1:B:378:HIS:ND1	1:B:382:ASP:OD2	2.48	0.45
1:B:18:THR:N	1:B:19:PRO:CD	2.80	0.43
1:A:10:TYR:HB3	1:A:59:GLU:HG2	2.00	0.43
1:B:481:PRO:HA	1:B:484:TRP:CD2	2.53	0.43
1:A:225:LEU:HD21	1:A:372:LEU:HD23	2.00	0.43
1:B:109:HIS:ND1	1:B:160:GLN:HB3	2.34	0.42
1:A:473:PHE:CE1	1:A:477:LYS:HG3	2.54	0.42
1:B:215:ARG:HD3	1:B:215:ARG:HA	1.91	0.42
1:B:435:ASN:C	1:B:435:ASN:HD22	2.23	0.42
1:A:353:ARG:HA	1:A:464:VAL:O	2.19	0.41
1:B:464:VAL:HG13	1:B:469:TRP:CE2	2.55	0.41
1:B:420:CYS:HB3	1:B:430:TRP:CE2	2.56	0.41
1:B:325:VAL:O	1:B:358:TRP:HA	2.20	0.41
1:B:225:LEU:HD21	1:B:372:LEU:HD22	2.03	0.40
1:A:73:ALA:HB2	6:A:2016:HOH:O	2.21	0.40
1:A:322:GLU:OE1	1:B:500:ARG:NH1	2.54	0.40
1:A:420:CYS:HB3	1:A:430:TRP:CE2	2.56	0.40
1:B:353:ARG:HA	1:B:464:VAL:O	2.22	0.40
1:A:279:TYR:CE1	1:B:246:MSE:HG2	2.57	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	471/522 (90%)	451 (96%)	19 (4%)	1 (0%)	52	59
1	B	486/522 (93%)	466 (96%)	18 (4%)	2 (0%)	39	42
All	All	957/1044 (92%)	917 (96%)	37 (4%)	3 (0%)	46	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	56	ASP
1	B	253	GLY
1	A	253	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	411/429 (96%)	399 (97%)	12 (3%)	50	62
1	B	418/429 (97%)	408 (98%)	10 (2%)	57	69
All	All	829/858 (97%)	807 (97%)	22 (3%)	52	64

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

Mol	Chain	Res	Type
1	A	131	LEU
1	A	149	LEU
1	A	151	LEU

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Mol	Chain	Res	Type
1	A	195	LEU
1	A	222	LEU
1	A	239	LEU
1	A	285	VAL
1	A	330	ARG
1	A	342	ILE
1	A	367	LYS
1	A	392	ARG
1	A	432	GLU
1	B	7	LEU
1	B	16	ASP
1	B	37	THR
1	B	47	LYS
1	B	113	MSE
1	B	170	LEU
1	B	195	LEU
1	B	363	GLU
1	B	432	GLU
1	B	435	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	B	320	ASN
1	B	435	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 6 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
4	ATP	A	1505	-	24,33,33	1.02	2 (8%)	31,52,52	1.76	5 (16%)
4	ATP	B	1507	5	24,33,33	0.99	2 (8%)	31,52,52	2.06	6 (19%)

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
4	ATP	A	1505	-	-	0/18/38/38	0/3/3/3
4	ATP	B	1507	5	-	0/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1507	ATP	O4'-C1'	2.01	1.43	1.41
4	A	1505	ATP	O4'-C1'	2.64	1.44	1.41
4	A	1505	ATP	C5-C4	2.96	1.47	1.40
4	B	1507	ATP	C5-C4	3.13	1.47	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1505	ATP	N3-C2-N1	-7.46	123.18	128.89
4	B	1507	ATP	N3-C2-N1	-7.14	123.43	128.89
4	B	1507	ATP	PA-O3A-PB	-4.29	120.67	132.73
4	B	1507	ATP	C2'-C1'-N9	-4.09	108.05	114.29
4	B	1507	ATP	PB-O3B-PG	-3.86	119.74	132.67
4	B	1507	ATP	C4-C5-N7	-2.89	106.82	109.48
4	A	1505	ATP	C2'-C1'-N9	-2.81	110.00	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	1505	ATP	C4-C5-N7	-2.44	107.24	109.48
4	A	1505	ATP	PB-O3B-PG	-2.17	125.39	132.67
4	A	1505	ATP	PA-O3A-PB	-2.15	126.69	132.73
4	B	1507	ATP	C2-N1-C6	2.15	122.61	118.77

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	464/522 (88%)	1.98	171 (36%)	0 0	55, 65, 140, 144	0
1	B	476/522 (91%)	1.55	129 (27%)	1 1	56, 64, 75, 95	0
All	All	940/1044 (90%)	1.76	300 (31%)	1 0	55, 64, 122, 144	0

All (300) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	161	TYR	11.6
1	B	165	ALA	11.1
1	A	86	GLY	10.8
1	A	25	ALA	10.5
1	B	58	ILE	10.4
1	B	163	ALA	10.2
1	A	161	TYR	10.0
1	A	96	ILE	9.8
1	A	74	ILE	9.8
1	A	163	ALA	9.2
1	A	164	LYS	9.0
1	A	11	PHE	9.0
1	A	167	HIS	8.9
1	A	165	ALA	8.5
1	B	15	ALA	8.4
1	A	87	LYS	8.3
1	A	-1	HIS	8.0
1	A	40	ALA	8.0
1	A	49	THR	7.4
1	A	-2	SER	7.3
1	B	164	LYS	7.2
1	B	162	GLY	7.2
1	B	167	HIS	7.1
1	B	95	GLY	7.1

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Mol	Chain	Res	Type	RSRZ
1	B	87	LYS	7.0
1	A	94	ARG	7.0
1	B	91	ILE	6.9
1	B	22	ASP	6.9
1	B	94	ARG	6.9
1	A	43	GLY	6.8
1	B	51	TRP	6.8
1	A	89	TYR	6.8
1	A	60	LEU	6.5
1	B	49	THR	6.4
1	A	28	PHE	6.4
1	A	162	GLY	6.3
1	B	92	GLY	6.3
1	B	13	THR	6.3
1	A	83	GLU	6.3
1	A	84	ALA	6.2
1	A	24	ILE	6.2
1	B	55	GLU	6.2
1	A	22	ASP	6.2
1	A	58	ILE	6.1
1	A	93	ILE	6.0
1	A	34	THR	6.0
1	A	27	LEU	6.0
1	A	131	LEU	6.0
1	B	79	LYS	5.9
1	A	91	ILE	5.9
1	A	101	PHE	5.8
1	A	51	TRP	5.8
1	A	105	VAL	5.8
1	A	77	LEU	5.6
1	A	160	GLN	5.5
1	A	109	HIS	5.5
1	A	126	GLU	5.5
1	B	82	ALA	5.5
1	A	92	GLY	5.5
1	A	108	ASP	5.2
1	A	7	LEU	5.2
1	B	57	ARG	5.2
1	A	41	PRO	5.2
1	B	275	VAL	5.2
1	B	290	ILE	5.2
1	B	166	GLU	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	36	LEU	5.1
1	A	128	GLY	5.0
1	A	81	LEU	5.0
1	A	119	ILE	5.0
1	A	70	VAL	4.9
1	A	166	GLU	4.9
1	A	110	GLU	4.9
1	A	57	ARG	4.8
1	A	9	ALA	4.8
1	B	90	LYS	4.8
1	B	14	SER	4.8
1	B	88	LYS	4.8
1	A	357	VAL	4.8
1	A	73	ALA	4.8
1	B	83	GLU	4.7
1	B	74	ILE	4.7
1	A	90	LYS	4.6
1	B	11	PHE	4.6
1	B	160	GLN	4.5
1	A	68	VAL	4.5
1	B	34	THR	4.5
1	A	23	ALA	4.4
1	A	33	SER	4.4
1	B	410	ASN	4.4
1	A	29	GLU	4.4
1	B	345	ILE	4.4
1	A	46	ALA	4.3
1	A	103	ILE	4.3
1	A	472	VAL	4.3
1	B	340	GLY	4.3
1	A	42	GLU	4.3
1	B	19	PRO	4.2
1	A	63	GLN	4.2
1	A	98	VAL	4.2
1	B	357	VAL	4.2
1	B	77	LEU	4.2
1	B	359	ILE	4.2
1	B	474	LEU	4.2
1	A	65	GLY	4.1
1	A	30	GLU	4.1
1	A	5	PHE	4.0
1	A	135	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	35	LEU	3.9
1	B	131	LEU	3.9
1	B	159	ALA	3.9
1	A	2	LYS	3.9
1	A	52	LYS	3.9
1	B	258	ILE	3.9
1	A	50	GLU	3.8
1	A	474	LEU	3.8
1	A	116	VAL	3.8
1	B	16	ASP	3.8
1	B	12	LYS	3.8
1	A	359	ILE	3.8
1	A	175	GLU	3.7
1	A	426	PRO	3.7
1	B	7	LEU	3.7
1	B	89	TYR	3.7
1	A	156	ILE	3.7
1	A	356	ILE	3.7
1	B	457	LEU	3.7
1	A	290	ILE	3.7
1	A	48	VAL	3.7
1	A	53	LEU	3.6
1	B	142	ASN	3.6
1	B	356	ILE	3.6
1	B	372	LEU	3.6
1	A	39	GLY	3.6
1	B	376	TYR	3.6
1	A	157	GLU	3.5
1	A	260	TYR	3.5
1	B	112	ARG	3.5
1	A	410	ASN	3.5
1	A	475	ALA	3.5
1	B	84	ALA	3.5
1	B	111	LEU	3.5
1	A	148	ILE	3.5
1	A	154	GLU	3.5
1	A	309	PHE	3.4
1	A	31	ALA	3.4
1	B	38	ARG	3.4
1	A	473	PHE	3.4
1	B	417	TYR	3.4
1	B	156	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	56	ASP	3.4
1	B	-3	GLY	3.4
1	A	66	ARG	3.4
1	A	436	VAL	3.4
1	B	168	TRP	3.3
1	A	376	TYR	3.3
1	B	325	VAL	3.3
1	A	470	ALA	3.3
1	B	342	ILE	3.3
1	A	168	TRP	3.3
1	A	393	VAL	3.3
1	B	50	GLU	3.3
1	A	120	LYS	3.3
1	B	28	PHE	3.3
1	B	24	ILE	3.3
1	B	103	ILE	3.2
1	A	67	TYR	3.2
1	B	143	ARG	3.2
1	B	109	HIS	3.2
1	B	239	LEU	3.2
1	A	427	ASP	3.2
1	A	159	ALA	3.2
1	A	38	ARG	3.1
1	A	384	LEU	3.1
1	A	71	HIS	3.1
1	A	255	TYR	3.1
1	B	358	TRP	3.1
1	B	29	GLU	3.1
1	A	104	LYS	3.0
1	A	10	TYR	3.0
1	A	345	ILE	3.0
1	A	62	LEU	3.0
1	A	245	TRP	3.0
1	B	225	LEU	3.0
1	A	85	LEU	3.0
1	A	310	TRP	3.0
1	B	348	VAL	3.0
1	A	240	VAL	2.9
1	A	88	LYS	2.9
1	B	133	LEU	2.9
1	A	213	ILE	2.9
1	B	148	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	133	LEU	2.9
1	A	142	ASN	2.9
1	B	436	VAL	2.9
1	B	380	PHE	2.9
1	A	178	GLU	2.9
1	A	79	LYS	2.9
1	B	10	TYR	2.9
1	B	30	GLU	2.9
1	A	75	PHE	2.8
1	B	60	LEU	2.8
1	B	205	ILE	2.8
1	A	26	ALA	2.8
1	A	372	LEU	2.8
1	B	386	ILE	2.8
1	B	96	ILE	2.8
1	B	431	LEU	2.8
1	B	33	SER	2.8
1	A	358	TRP	2.8
1	B	310	TRP	2.7
1	B	472	VAL	2.7
1	B	360	GLY	2.7
1	A	236	PHE	2.7
1	B	471	ALA	2.7
1	A	392	ARG	2.7
1	A	386	ILE	2.6
1	B	339	SER	2.6
1	B	488	PHE	2.6
1	A	134	GLU	2.6
1	B	327	VAL	2.6
1	B	194	TRP	2.6
1	A	235	ILE	2.6
1	A	417	TYR	2.6
1	A	95	GLY	2.6
1	A	471	ALA	2.6
1	B	158	ALA	2.6
1	A	419	ALA	2.6
1	B	81	LEU	2.6
1	A	176	PRO	2.6
1	A	306	CYS	2.6
1	B	415	THR	2.6
1	A	78	ARG	2.5
1	A	37	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	393	VAL	2.5
1	B	379	ILE	2.5
1	B	21	LYS	2.5
1	A	459	SER	2.5
1	B	459	SER	2.5
1	B	484	TRP	2.5
1	A	152	LEU	2.5
1	A	202	GLY	2.5
1	B	93	ILE	2.5
1	A	348	VAL	2.4
1	A	12	LYS	2.4
1	B	31	ALA	2.4
1	A	129	ILE	2.4
1	B	105	VAL	2.4
1	B	479	LEU	2.4
1	B	110	GLU	2.4
1	B	245	TRP	2.4
1	A	69	ARG	2.4
1	B	473	PHE	2.4
1	A	59	GLU	2.4
1	A	380	PHE	2.4
1	A	488	PHE	2.4
1	A	197[A]	ARG	2.4
1	A	327	VAL	2.4
1	B	98	VAL	2.4
1	B	20	ALA	2.3
1	A	261	VAL	2.3
1	A	275	VAL	2.3
1	B	85	LEU	2.3
1	A	313	VAL	2.3
1	B	341	GLY	2.3
1	B	132	GLU	2.3
1	A	127	GLY	2.3
1	B	388	TRP	2.2
1	A	82	ALA	2.2
1	B	178	GLU	2.2
1	A	61	THR	2.2
1	A	312	TYR	2.2
1	A	429	GLU	2.2
1	B	285	VAL	2.2
1	A	259	TYR	2.2
1	B	384	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	427	ASP	2.1
1	A	111	LEU	2.1
1	A	460	GLY	2.1
1	A	476	GLN	2.1
1	B	451	LEU	2.1
1	B	302	CYS	2.1
1	A	204	TRP	2.1
1	A	438	ILE	2.1
1	B	213	ILE	2.1
1	B	351	PHE	2.1
1	A	239	LEU	2.1
1	A	500	ARG	2.1
1	B	323	ILE	2.1
1	A	225	LEU	2.1
1	A	339	SER	2.1
1	A	294	ILE	2.1
1	A	281	VAL	2.1
1	B	235	ILE	2.0
1	A	76	ARG	2.0
1	B	86	GLY	2.0
1	B	152	LEU	2.0
1	A	136	GLY	2.0
1	B	300	GLY	2.0
1	B	336	ARG	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
4	ATP	A	1505	31/31	0.90	0.24	1.17	41,47,65,66	0
4	ATP	B	1507	31/31	0.87	0.23	0.20	49,58,78,78	0
3	CL	B	1504	1/1	0.98	0.12	-1.91	37,37,37,37	0
3	CL	A	1504	1/1	0.99	0.12	-2.06	34,34,34,34	0
2	ZN	B	1503	1/1	0.99	0.04	-	44,44,44,44	0
5	MG	B	1506	1/1	0.72	0.57	-	76,76,76,76	0
2	ZN	A	1503	1/1	0.99	0.04	-	39,39,39,39	0
5	MG	B	1505	1/1	0.88	0.14	-	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.