



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:01 PM UTC

PDB ID : 5WS4 / pdb_00005ws4
Title : Crystal structure of tripartite-type ABC transporter MacB from *Acinetobacter baumannii*
Authors : Murakami, S.; Okada, U.; Yamashita, E.
Deposited on : 2016-12-05
Resolution : 3.40 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

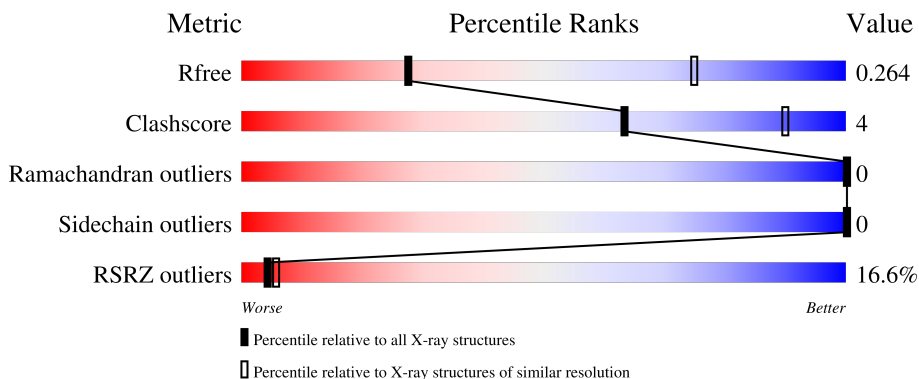
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	671	14% 85% 11% .
1	B	671	18% 87% 9% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9824 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.

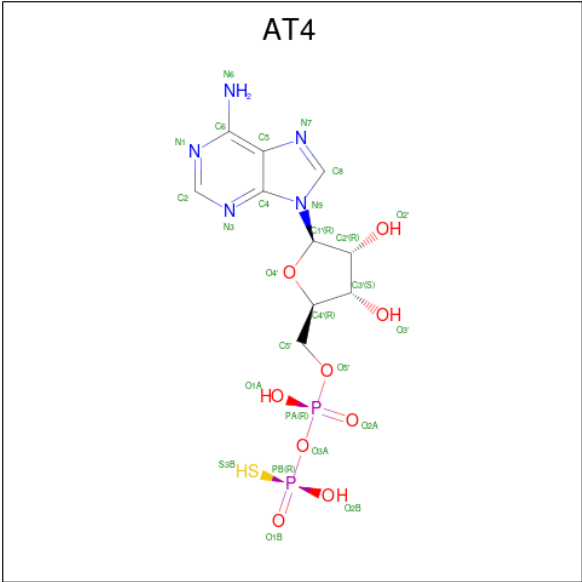
- Molecule 1 is a protein called Macrolide export ATP-binding/permease protein MacB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	650	Total	C	N	O	S	0	0	0
			4885	3056	854	952	23			
1	B	650	Total	C	N	O	S	0	0	0
			4885	3056	854	952	23			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	expression tag	UNP A0A0D8G707
A	-5	HIS	-	expression tag	UNP A0A0D8G707
A	-4	HIS	-	expression tag	UNP A0A0D8G707
A	-3	HIS	-	expression tag	UNP A0A0D8G707
A	-2	HIS	-	expression tag	UNP A0A0D8G707
A	-1	HIS	-	expression tag	UNP A0A0D8G707
A	0	HIS	-	expression tag	UNP A0A0D8G707
B	-6	MET	-	expression tag	UNP A0A0D8G707
B	-5	HIS	-	expression tag	UNP A0A0D8G707
B	-4	HIS	-	expression tag	UNP A0A0D8G707
B	-3	HIS	-	expression tag	UNP A0A0D8G707
B	-2	HIS	-	expression tag	UNP A0A0D8G707
B	-1	HIS	-	expression tag	UNP A0A0D8G707
B	0	HIS	-	expression tag	UNP A0A0D8G707

- Molecule 2 is 5'-O-[(R)-HYDROXY(THIOPHOSPHONOOXY)PHOSPHORYL]ADENOSINE (CCD ID: AT4) (formula: C₁₀H₁₅N₅O₉P₂S).

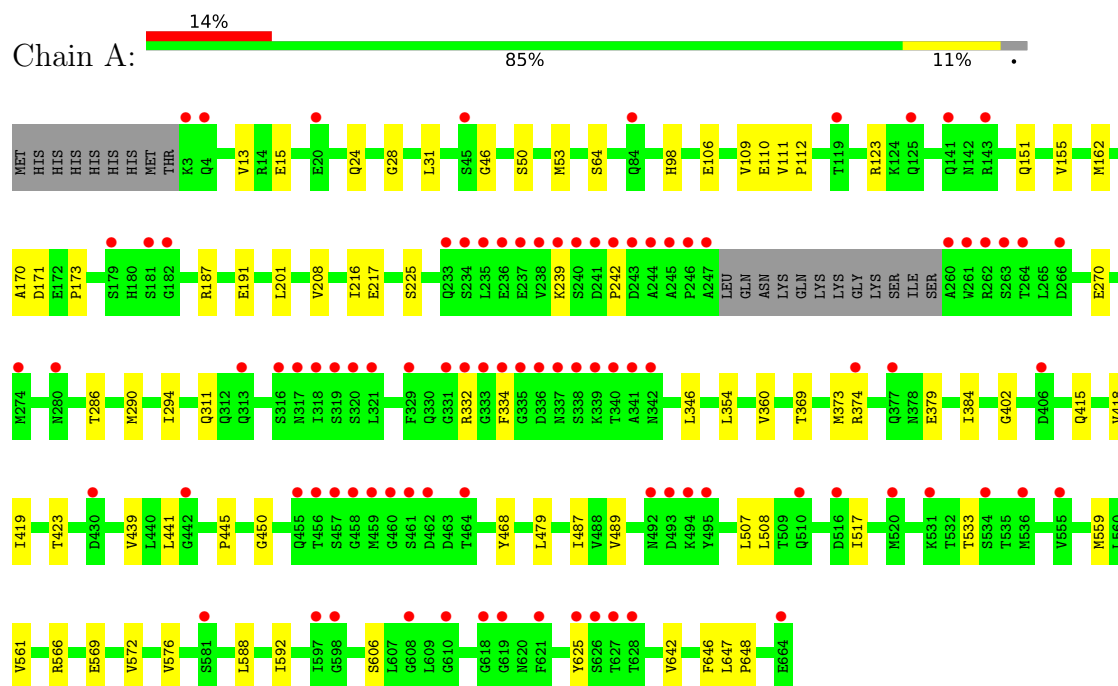


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	A	1	Total 27	C 10	N 5	O 9	P 2	S 1	0	0
2	B	1	Total 27	C 10	N 5	O 9	P 2	S 1	0	0

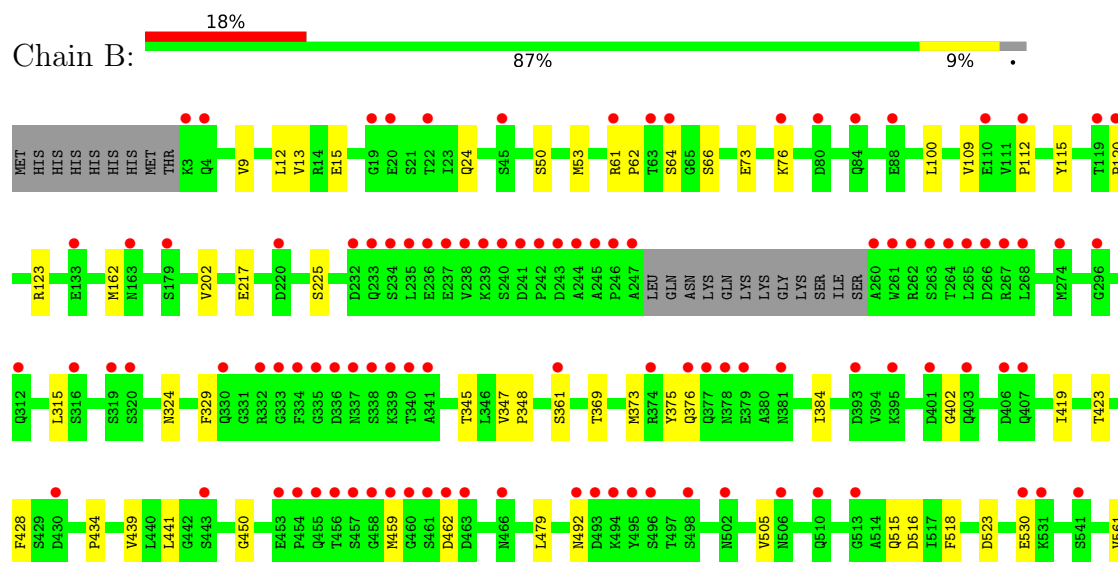
3 Residue-property plots [i](#)

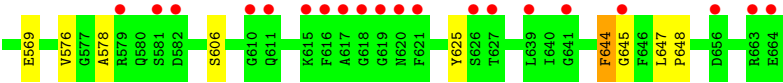
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Macrolide export ATP-binding/permease protein MacB



- Molecule 1: Macrolide export ATP-binding/permease protein MacB





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	229.65Å 229.65Å 154.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.12 – 3.40 49.12 – 3.40	Depositor EDS
% Data completeness (in resolution range)	81.2 (49.12-3.40) 81.3 (49.12-3.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.227 , 0.257 0.235 , 0.264	Depositor DCC
R_{free} test set	2357 reflections (4.02%)	wwPDB-VP
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	9824	wwPDB-VP
Average B, all atoms (Å ²)	62.0	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 39.62 % 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 3.0907e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AT4

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	0.19	0/4945	0.51	0/6703
1	B	0.18	0/4945	0.50	6/6703 (0.1%)
All	All	0.19	0/9890	0.50	6/13406 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	462	ASP	CA-C-N	5.53	131.66	121.70
1	B	462	ASP	C-N-CA	5.53	131.66	121.70
1	B	644	PHE	CA-C-N	5.16	130.99	121.70
1	B	644	PHE	C-N-CA	5.16	130.99	121.70
1	B	62	PRO	CA-C-N	5.15	131.38	121.54
1	B	62	PRO	C-N-CA	5.15	131.38	121.54

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	4885	0	4973	45	0
1	B	4885	0	4973	35	0
2	A	27	0	13	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	27	0	13	2	0
All	All	9824	0	9972	80	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 4.

All (80) 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:53:MET:HE1	1:A:171:ASP:HB2	1.60	0.83
1:B:50:SER:OG	2:B:701:AT4:O5'	2.03	0.76
1:B:324:ASN:ND2	1:B:523:ASP:OD2	2.22	0.72
1:B:13:VAL:HB	1:B:64:SER:HB3	1.70	0.71
1:A:402:GLY:HA3	1:A:450:GLY:HA2	1.77	0.67
1:A:13:VAL:HB	1:A:64:SER:HB3	1.76	0.67
1:A:286:THR:HG22	1:A:290:MET:HE2	1.80	0.63
1:A:15:GLU:HG2	1:A:24:GLN:HG2	1.81	0.63
1:A:170:ALA:HB1	1:A:173:PRO:HG3	1.80	0.63
1:B:369:THR:HB	1:B:479:LEU:HD21	1.81	0.63
1:B:644:PHE:N	1:B:645:GLY:HA3	2.15	0.61
1:A:217:GLU:HB3	1:A:225:SER:HB3	1.83	0.60
1:B:345:THR:OG1	1:B:516:ASP:OD2	2.21	0.58
1:B:402:GLY:HA3	1:B:450:GLY:HA2	1.87	0.57
1:B:9:VAL:HG13	1:B:12:LEU:HG	1.87	0.56
1:B:109:VAL:HG12	1:B:162:MET:HE2	1.88	0.56
1:A:170:ALA:HB1	1:A:173:PRO:CG	2.36	0.55
1:A:109:VAL:HG12	1:A:162:MET:HE2	1.89	0.55
1:A:187:ARG:NH1	1:A:191:GLU:OE2	2.39	0.55
1:B:217:GLU:HB3	1:B:225:SER:HB3	1.90	0.53
1:B:606:SER:O	1:B:625:TYR:OH	2.21	0.53
1:A:112:PRO:HG3	1:A:576:VAL:HB	1.90	0.53
1:A:123:ARG:NH2	1:A:270:GLU:OE2	2.37	0.52
1:A:374:ARG:HG2	1:A:379:GLU:HG2	1.92	0.52
1:A:13:VAL:HG22	1:A:28:GLY:H	1.75	0.52
1:A:369:THR:HB	1:A:479:LEU:HD21	1.92	0.51
1:B:100:LEU:HD22	1:B:569:GLU:HG3	1.92	0.51
1:A:201:LEU:HD21	1:A:208:VAL:HG12	1.94	0.50
1:B:361:SER:HB3	1:B:492:ASN:HB3	1.94	0.49
1:A:50:SER:OG	2:A:801:AT4:O5'	2.30	0.49
1:A:98:HIS:HB3	1:A:572:VAL:HG21	1.96	0.48
1:A:46:GLY:HA2	2:A:801:AT4:O3'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:PRO:HB3	1:B:576:VAL:HG13	1.95	0.48
1:A:354:LEU:HD23	1:A:507:LEU:HD23	1.95	0.47
1:B:329:PHE:HB2	1:B:518:PHE:CE2	2.49	0.47
1:A:106:GLU:O	1:A:110:GLU:HG3	2.14	0.47
1:A:419:ILE:HB	1:A:423:THR:OG1	2.14	0.47
2:B:701:AT4:H5'2	2:B:701:AT4:H8	1.97	0.47
1:A:508:LEU:HB2	1:A:517:ILE:HD13	1.96	0.47
1:B:115:TYR:CZ	1:B:578:ALA:HB2	2.50	0.47
1:B:315:LEU:HD11	1:B:530:GLU:HG2	1.97	0.47
1:B:120:PRO:O	1:B:123:ARG:HG2	2.15	0.46
1:A:647:LEU:HB3	1:A:648:PRO:HD3	1.97	0.46
1:B:384:ILE:HD11	1:B:441:LEU:HB3	1.97	0.45
1:B:15:GLU:HG2	1:B:24:GLN:HG2	1.96	0.45
1:B:428:PHE:CG	1:B:434:PRO:HG3	2.52	0.45
1:A:642:VAL:O	1:A:646:PHE:HB2	2.16	0.45
1:B:419:ILE:HB	1:B:423:THR:OG1	2.17	0.45
1:A:332:ARG:HG3	1:B:515:GLN:NE2	2.32	0.44
1:B:347:VAL:HB	1:B:348:PRO:HD2	1.99	0.44
1:B:505:VAL:HG11	1:B:515:GLN:HE22	1.82	0.44
1:B:53:MET:HE3	1:B:53:MET:HB3	1.93	0.44
1:B:66:SER:OG	1:B:73:GLU:OE1	2.30	0.44
1:A:290:MET:O	1:A:294:ILE:HG13	2.18	0.44
1:A:373:MET:HE3	1:A:439:VAL:HG21	1.99	0.44
2:A:801:AT4:H4'	2:A:801:AT4:O1A	2.16	0.44
1:A:566:ARG:HD2	1:A:569:GLU:OE1	2.18	0.44
1:A:588:LEU:HD13	1:A:646:PHE:HA	1.99	0.44
1:B:53:MET:HB2	1:B:202:VAL:HG21	2.00	0.44
1:A:311:GLN:HB2	1:A:533:THR:HG21	1.99	0.44
1:A:592:ILE:HD11	1:A:642:VAL:HG22	2.00	0.44
1:B:647:LEU:HB3	1:B:648:PRO:HD3	2.00	0.43
1:B:61:ARG:HH21	1:B:76:LYS:HA	1.82	0.43
1:B:375:TYR:O	1:B:376:GLN:C	2.62	0.43
1:A:31:LEU:HD11	1:A:216:ILE:HD13	2.00	0.42
1:B:373:MET:HE3	1:B:439:VAL:HG21	2.01	0.42
1:A:360:VAL:HG13	1:A:489:VAL:HG13	2.02	0.42
1:B:459:MET:HE2	1:B:459:MET:HA	2.02	0.42
1:A:561:VAL:HG11	1:B:561:VAL:HG11	2.01	0.42
1:A:239:LYS:HE2	1:A:242:PRO:HA	2.01	0.42
1:A:384:ILE:HD11	1:A:441:LEU:HB3	2.02	0.41
1:A:415:GLN:NE2	1:A:445:PRO:O	2.46	0.41
1:A:559:MET:HE3	1:A:559:MET:HB3	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:VAL:HB	1:A:112:PRO:HD3	2.02	0.41
1:A:418:VAL:HB	1:A:468:TYR:HB2	2.03	0.41
1:A:151:GLN:O	1:A:155:VAL:HG23	2.21	0.41
1:A:606:SER:O	1:A:625:TYR:OH	2.24	0.41
1:A:334:PHE:CD1	1:A:334:PHE:N	2.88	0.40
1:B:9:VAL:CG1	1:B:12:LEU:HG	2.50	0.40
1:A:346:LEU:HD11	1:A:487:ILE:HD12	2.04	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	646/671 (96%)	616 (95%)	30 (5%)	0	100	100
1	B	646/671 (96%)	618 (96%)	28 (4%)	0	100	100
All	All	1292/1342 (96%)	1234 (96%)	58 (4%)	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	538/558 (96%)	538 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	538/558 (96%)	538 (100%)	0	100	100
All	All	1076/1116 (96%)	1076 (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 (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	HIS
1	A	357	GLN
1	A	385	ASN
1	A	455	GLN
1	A	483	HIS
1	B	207	GLN
1	B	233	GLN
1	B	385	ASN
1	B	389	ASN
1	B	455	GLN
1	B	515	GLN
1	B	586	GLN

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	AT4	B	701	-	27,29,29	3.33	15 (55%)	39,45,45	2.55	16 (41%)
2	AT4	A	801	-	27,29,29	3.21	13 (48%)	39,45,45	2.58	17 (43%)

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	AT4	B	701	-	-	4/14/32/32	0/3/3/3
2	AT4	A	801	-	-	4/14/32/32	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	AT4	C2'-C3'	-9.11	1.28	1.53
2	A	801	AT4	C2'-C3'	-9.09	1.28	1.53
2	A	801	AT4	O4'-C4'	-6.89	1.29	1.45
2	B	701	AT4	O4'-C4'	-6.81	1.29	1.45
2	A	801	AT4	O4'-C1'	4.97	1.53	1.42
2	B	701	AT4	O4'-C1'	4.94	1.53	1.42
2	B	701	AT4	PA-O3A	4.80	1.64	1.59
2	A	801	AT4	PA-O3A	4.56	1.64	1.59
2	B	701	AT4	PB-O1B	4.32	1.56	1.46
2	A	801	AT4	C6-N6	4.17	1.44	1.34
2	B	701	AT4	C6-N6	4.16	1.44	1.34
2	B	701	AT4	C1'-N9	-3.94	1.35	1.46
2	A	801	AT4	C1'-N9	-3.86	1.35	1.46
2	B	701	AT4	C3'-C4'	3.65	1.62	1.53
2	A	801	AT4	C3'-C4'	3.62	1.62	1.53
2	B	701	AT4	C5-C4	-3.30	1.33	1.39
2	A	801	AT4	C5-C4	-3.25	1.33	1.39
2	A	801	AT4	O2'-C2'	2.80	1.49	1.43
2	B	701	AT4	O2'-C2'	2.67	1.49	1.43
2	A	801	AT4	PA-O5'	2.59	1.69	1.59
2	B	701	AT4	PA-O5'	2.55	1.69	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	AT4	C8-N9	-2.43	1.33	1.37
2	A	801	AT4	C5-N7	-2.42	1.34	1.39
2	B	701	AT4	C8-N9	-2.41	1.33	1.37
2	B	701	AT4	C5-N7	-2.36	1.34	1.39
2	A	801	AT4	PB-O1B	2.25	1.51	1.46
2	B	701	AT4	PB-O2B	-2.23	1.51	1.56
2	B	701	AT4	C4-N9	-2.04	1.33	1.37

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	AT4	N6-C6-N1	-6.33	104.28	118.38
2	A	801	AT4	N6-C6-N1	-6.24	104.48	118.38
2	A	801	AT4	N3-C2-N1	-5.70	119.96	128.58
2	B	701	AT4	N3-C2-N1	-5.63	120.05	128.58
2	B	701	AT4	C5-C6-N6	5.19	136.15	123.29
2	A	801	AT4	C5-C6-N6	5.11	135.93	123.29
2	B	701	AT4	N9-C8-N7	-4.49	107.57	113.94
2	A	801	AT4	N9-C8-N7	-4.36	107.76	113.94
2	A	801	AT4	C5-C4-N3	-4.24	120.88	126.72
2	B	701	AT4	C5-C4-N3	-4.13	121.02	126.72
2	B	701	AT4	C5'-C4'-C3'	-3.98	100.87	115.21
2	A	801	AT4	C1'-N9-C8	-3.65	118.99	127.09
2	A	801	AT4	C5'-C4'-C3'	-3.65	102.08	115.21
2	B	701	AT4	C2'-C3'-C4'	3.47	109.31	102.61
2	B	701	AT4	C1'-N9-C8	-3.47	119.40	127.09
2	A	801	AT4	C2'-C3'-C4'	3.40	109.19	102.61
2	A	801	AT4	C2-N3-C4	3.25	119.78	111.83
2	B	701	AT4	C2-N3-C4	3.17	119.57	111.83
2	A	801	AT4	C3'-C2'-C1'	3.05	107.23	101.46
2	B	701	AT4	C3'-C2'-C1'	2.91	106.97	101.46
2	B	701	AT4	C4-N9-C8	2.86	108.75	105.74
2	B	701	AT4	C5-N7-C8	2.79	107.84	103.45
2	A	801	AT4	C5-N7-C8	2.73	107.74	103.45
2	A	801	AT4	C4-N9-C8	2.69	108.56	105.74
2	A	801	AT4	C4-N9-C1'	2.49	132.45	126.63
2	A	801	AT4	N3-C4-N9	2.38	131.22	127.17
2	B	701	AT4	N3-C4-N9	2.32	131.11	127.17
2	A	801	AT4	O4'-C4'-C3'	2.31	109.74	105.15
2	B	701	AT4	C4-C5-N7	-2.27	107.98	110.58
2	A	801	AT4	O1A-PA-O3A	2.24	113.33	107.27
2	B	701	AT4	C4-N9-C1'	2.23	131.85	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	AT4	C4-C5-N7	-2.22	108.04	110.58
2	B	701	AT4	O4'-C4'-C3'	2.20	109.52	105.15

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	AT4	C4'-C5'-O5'-PA
2	B	701	AT4	C4'-C5'-O5'-PA
2	B	701	AT4	O4'-C4'-C5'-O5'
2	A	801	AT4	C3'-C4'-C5'-O5'
2	A	801	AT4	O4'-C4'-C5'-O5'
2	B	701	AT4	C3'-C4'-C5'-O5'
2	A	801	AT4	PB-O3A-PA-O5'
2	B	701	AT4	PB-O3A-PA-O5'

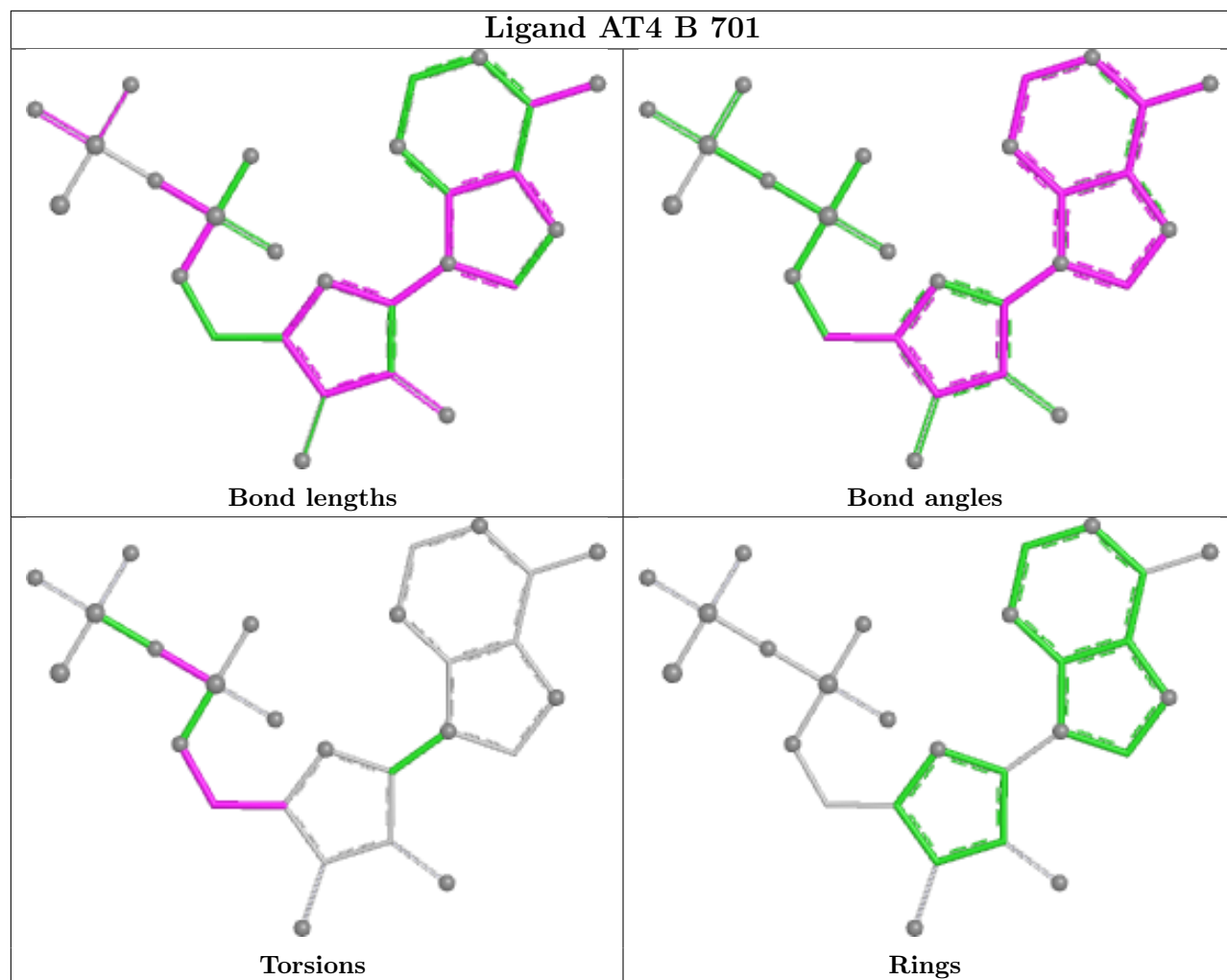
There are no ring outliers.

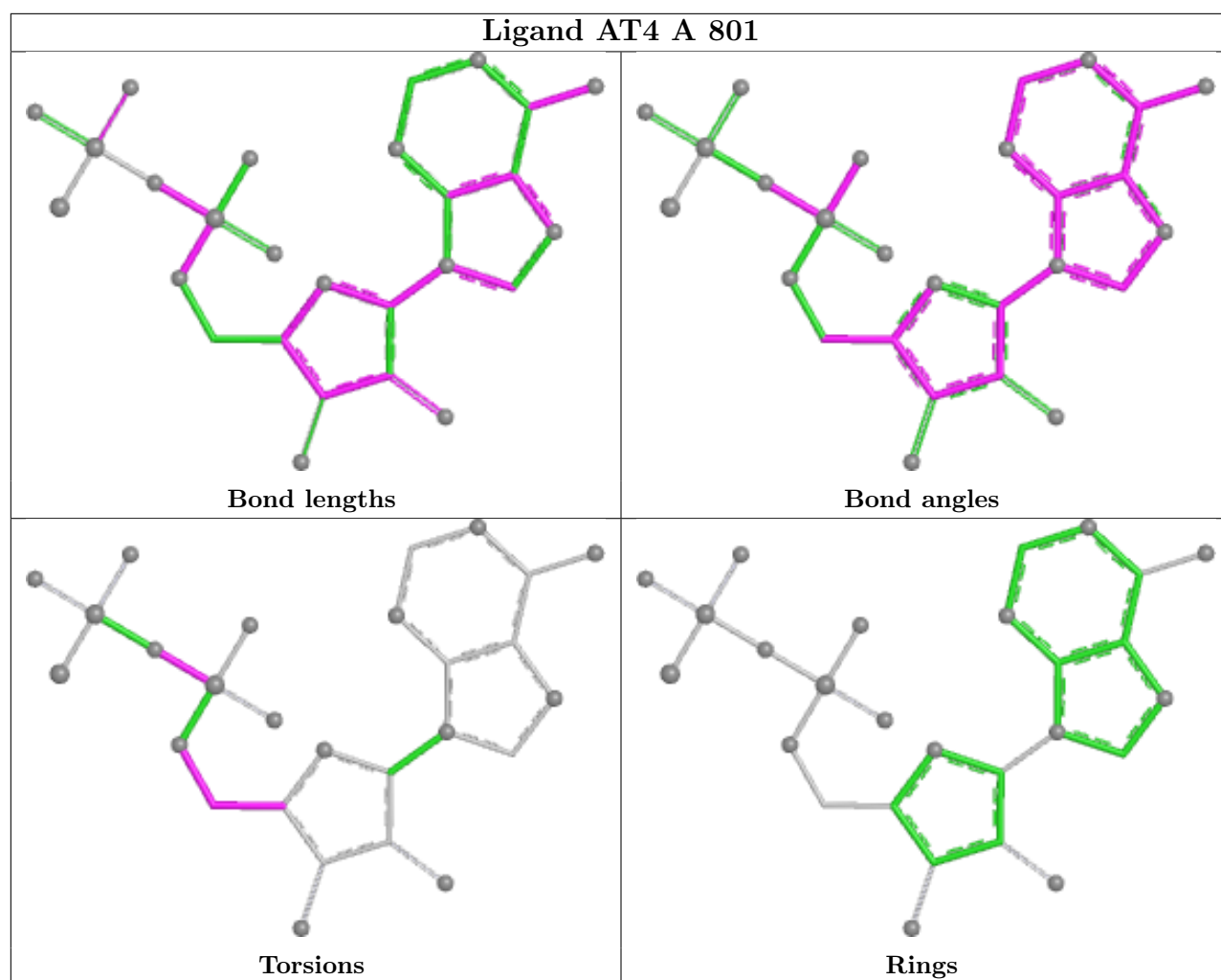
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	AT4	2	0
2	A	801	AT4	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand AT4 B 701





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	650/671 (96%)	0.85	93 (14%) 6 8	17, 49, 125, 184	0
1	B	650/671 (96%)	1.18	123 (18%) 3 4	21, 60, 142, 180	0
All	All	1300/1342 (96%)	1.01	216 (16%) 4 6	17, 55, 134, 184	0

All (216) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	334	PHE	15.4
1	B	617	ALA	12.0
1	A	261	TRP	10.1
1	A	334	PHE	9.6
1	B	260	ALA	9.3
1	B	456	THR	8.8
1	B	333	GLY	8.7
1	B	242	PRO	8.3
1	B	261	TRP	8.0
1	B	457	SER	8.0
1	A	260	ALA	7.6
1	A	239	LYS	7.5
1	A	238	VAL	7.5
1	B	337	ASN	7.3
1	B	238	VAL	7.3
1	B	495	TYR	7.0
1	B	163	ASN	6.9
1	A	339	LYS	6.7
1	B	460	GLY	6.6
1	B	341	ALA	6.4
1	B	338	SER	6.4
1	B	401	ASP	6.2
1	B	493	ASP	6.2
1	A	242	PRO	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	493	ASP	6.1
1	A	457	SER	6.0
1	B	240	SER	5.9
1	B	461	SER	5.8
1	B	335	GLY	5.7
1	B	245	ALA	5.6
1	A	495	TYR	5.6
1	A	340	THR	5.5
1	B	618	GLY	5.4
1	A	456	THR	5.4
1	B	239	LYS	5.4
1	A	338	SER	5.2
1	B	332	ARG	5.2
1	A	235	LEU	5.1
1	A	664	GLU	5.1
1	A	461	SER	5.1
1	A	619	GLY	5.1
1	A	464	THR	5.1
1	A	342	ASN	5.0
1	A	263	SER	5.0
1	B	235	LEU	5.0
1	A	240	SER	4.9
1	B	263	SER	4.9
1	A	333	GLY	4.9
1	B	458	GLY	4.9
1	B	339	LYS	4.9
1	B	274	MET	4.9
1	A	266	ASP	4.9
1	B	336	ASP	4.8
1	B	267	ARG	4.8
1	B	620	ASN	4.7
1	A	237	GLU	4.6
1	B	494	LYS	4.6
1	A	459	MET	4.6
1	B	616	PHE	4.5
1	B	266	ASP	4.4
1	A	262	ARG	4.3
1	B	459	MET	4.3
1	B	455	GLN	4.3
1	A	245	ALA	4.2
1	B	264	THR	4.2
1	A	628	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	458	GLY	4.1
1	A	246	PRO	4.1
1	B	119	THR	4.0
1	B	377	GLN	4.0
1	B	244	ALA	3.9
1	A	316	SER	3.9
1	A	236	GLU	3.9
1	B	234	SER	3.9
1	B	120	PRO	3.8
1	A	179	SER	3.8
1	A	331	GLY	3.8
1	A	627	THR	3.8
1	B	531	LYS	3.7
1	A	125	GLN	3.7
1	B	20	GLU	3.7
1	A	274	MET	3.7
1	A	455	GLN	3.6
1	B	407	GLN	3.6
1	A	244	ALA	3.6
1	B	506	ASN	3.6
1	B	45	SER	3.6
1	A	241	ASP	3.6
1	B	3	LYS	3.5
1	B	619	GLY	3.5
1	A	531	LYS	3.5
1	B	510	GLN	3.5
1	B	61	ARG	3.5
1	B	579	ARG	3.4
1	A	3	LYS	3.4
1	B	664	GLU	3.4
1	A	313	GLN	3.4
1	A	516	ASP	3.4
1	B	312	GLN	3.4
1	B	376	GLN	3.4
1	B	76	LYS	3.4
1	A	20	GLU	3.4
1	A	460	GLY	3.4
1	B	627	THR	3.3
1	A	337	ASN	3.3
1	A	336	ASP	3.3
1	B	582	ASP	3.3
1	A	335	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	243	ASP	3.3
1	B	406	ASP	3.3
1	A	462	ASP	3.2
1	B	615	LYS	3.2
1	B	262	ARG	3.2
1	B	237	GLU	3.2
1	B	246	PRO	3.2
1	A	234	SER	3.2
1	A	319	SER	3.2
1	B	393	ASP	3.2
1	B	179	SER	3.1
1	A	317	ASN	3.1
1	B	454	PRO	3.1
1	A	341	ALA	3.1
1	B	621	PHE	3.1
1	B	19	GLY	3.1
1	A	492	ASN	3.0
1	B	4	GLN	3.0
1	A	247	ALA	3.0
1	A	318	ILE	3.0
1	B	84	GLN	3.0
1	B	492	ASN	3.0
1	B	63	THR	3.0
1	A	430	ASP	2.9
1	A	406	ASP	2.9
1	B	462	ASP	2.9
1	B	443	SER	2.9
1	B	233	GLN	2.9
1	A	329	PHE	2.9
1	B	320	SER	2.8
1	B	243	ASP	2.8
1	A	536	MET	2.8
1	B	374	ARG	2.8
1	A	280	ASN	2.8
1	B	645	GLY	2.8
1	A	45	SER	2.8
1	A	626	SER	2.8
1	A	494	LYS	2.8
1	B	453	GLU	2.8
1	A	621	PHE	2.7
1	A	332	ARG	2.7
1	B	296	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	639	LEU	2.7
1	B	64	SER	2.7
1	A	264	THR	2.6
1	A	320	SER	2.6
1	B	403	GLN	2.6
1	B	340	THR	2.6
1	A	510	GLN	2.6
1	B	378	ASN	2.6
1	B	265	LEU	2.6
1	B	220	ASP	2.6
1	B	241	ASP	2.6
1	B	611	GLN	2.5
1	A	182	GLY	2.5
1	B	496	SER	2.5
1	B	236	GLU	2.5
1	A	442	GLY	2.5
1	B	663	ARG	2.5
1	A	181	SER	2.5
1	A	143	ARG	2.5
1	A	321	LEU	2.5
1	A	377	GLN	2.5
1	B	316	SER	2.4
1	B	626	SER	2.4
1	B	581	SER	2.4
1	A	581	SER	2.4
1	B	541	SER	2.4
1	B	513	GLY	2.4
1	B	430	ASP	2.4
1	A	374	ARG	2.4
1	A	4	GLN	2.4
1	B	268	LEU	2.4
1	A	618	GLY	2.3
1	B	112	PRO	2.3
1	A	119	THR	2.3
1	A	141	GLN	2.3
1	B	133	GLU	2.3
1	B	610	GLY	2.3
1	B	466	ASN	2.3
1	A	610	GLY	2.3
1	A	84	GLN	2.3
1	B	88	GLU	2.3
1	A	520	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	232	ASP	2.2
1	B	463	ASP	2.2
1	A	625	TYR	2.2
1	B	530	GLU	2.2
1	B	395	LYS	2.2
1	A	598	GLY	2.2
1	B	247	ALA	2.2
1	B	80	ASP	2.2
1	B	379	GLU	2.1
1	B	22	THR	2.1
1	B	330	GLN	2.1
1	B	381	ASN	2.1
1	B	641	GLY	2.1
1	B	319	SER	2.1
1	B	498	SER	2.1
1	A	233	GLN	2.1
1	A	608	GLY	2.1
1	A	534	SER	2.1
1	A	597	ILE	2.0
1	B	502	ASN	2.0
1	B	110	GLU	2.0
1	A	555	VAL	2.0
1	B	361	SER	2.0
1	B	656	ASP	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](#)

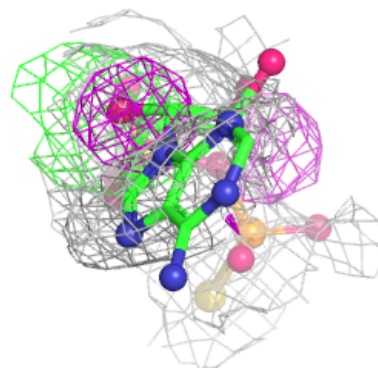
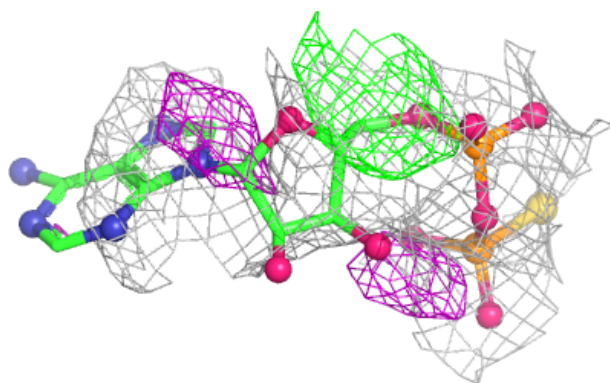
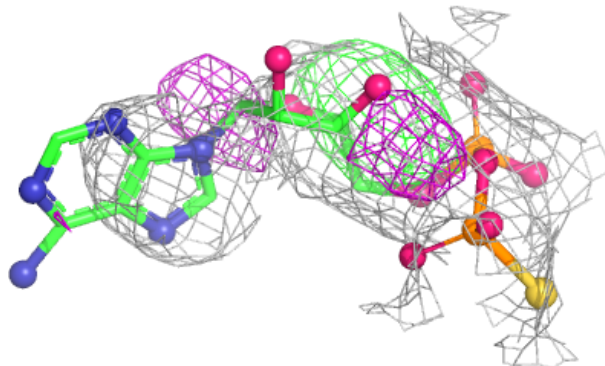
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	AT4	B	701	27/27	0.79	0.24	126,141,182,190	0
2	AT4	A	801	27/27	0.80	0.24	99,111,168,180	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

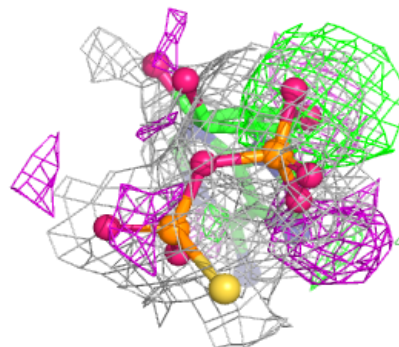
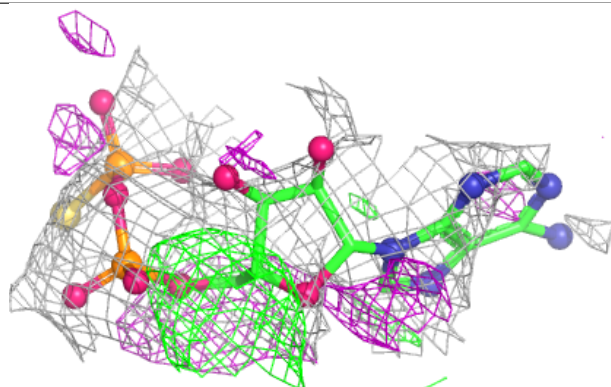
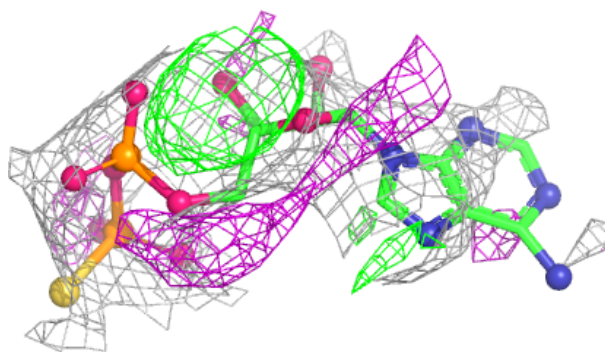
Electron density around AT4 B 701:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around AT4 A 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.