



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:40 PM UTC

PDB ID : 3UE0 / pdb_00003ue0
Title : Crystal structure of Acinetobacter baumannii PBP1a in complex with Aztreonam
Authors : Han, S.
Deposited on : 2011-10-28
Resolution : 2.60 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

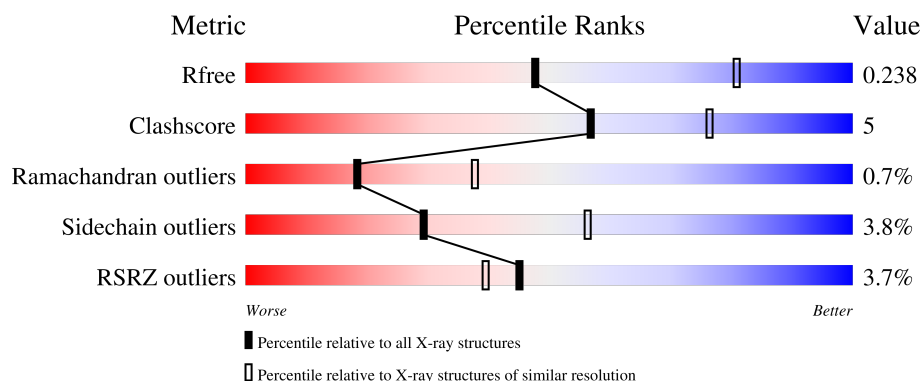
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

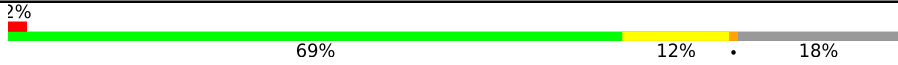
The reported resolution of this entry is 2.60 Å.

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	731	
1	B	731	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9762 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 Penicillin-binding protein 1a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	598	Total	C	N	O	S	0	0	0
			4715	3006	832	861	16			
1	B	595	Total	C	N	O	S	0	0	0
			4684	2986	826	856	16			

There are 32 discrepancies between the modelled and reference sequences:

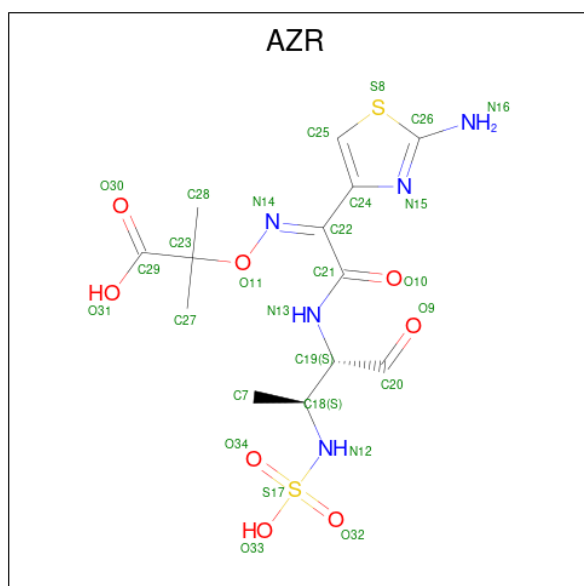
Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	expression tag	UNP G1C794
A	10	HIS	-	expression tag	UNP G1C794
A	11	HIS	-	expression tag	UNP G1C794
A	12	HIS	-	expression tag	UNP G1C794
A	13	HIS	-	expression tag	UNP G1C794
A	14	HIS	-	expression tag	UNP G1C794
A	15	HIS	-	expression tag	UNP G1C794
A	16	GLU	-	expression tag	UNP G1C794
A	17	ASN	-	expression tag	UNP G1C794
A	18	LEU	-	expression tag	UNP G1C794
A	19	TYR	-	expression tag	UNP G1C794
A	20	PHE	-	expression tag	UNP G1C794
A	21	GLN	-	expression tag	UNP G1C794
A	22	SER	-	expression tag	UNP G1C794
A	23	HIS	-	expression tag	UNP G1C794
A	24	MET	-	expression tag	UNP G1C794
B	9	MET	-	expression tag	UNP G1C794
B	10	HIS	-	expression tag	UNP G1C794
B	11	HIS	-	expression tag	UNP G1C794
B	12	HIS	-	expression tag	UNP G1C794
B	13	HIS	-	expression tag	UNP G1C794
B	14	HIS	-	expression tag	UNP G1C794
B	15	HIS	-	expression tag	UNP G1C794
B	16	GLU	-	expression tag	UNP G1C794
B	17	ASN	-	expression tag	UNP G1C794

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Chain	Residue	Modelled	Actual	Comment	Reference
B	18	LEU	-	expression tag	UNP G1C794
B	19	TYR	-	expression tag	UNP G1C794
B	20	PHE	-	expression tag	UNP G1C794
B	21	GLN	-	expression tag	UNP G1C794
B	22	SER	-	expression tag	UNP G1C794
B	23	HIS	-	expression tag	UNP G1C794
B	24	MET	-	expression tag	UNP G1C794

- Molecule 2 is 2-({[(1Z)-1-(2-amino-1,3-thiazol-4-yl)-2-oxo-2-{[(2S,3S)-1-oxo-3-(sulfoamino)butan-2-yl]amino}ethylidene]amino}oxy)-2-methylpropanoic acid (CCD ID: AZR) (formula: $C_{13}H_{19}N_5O_8S_2$).



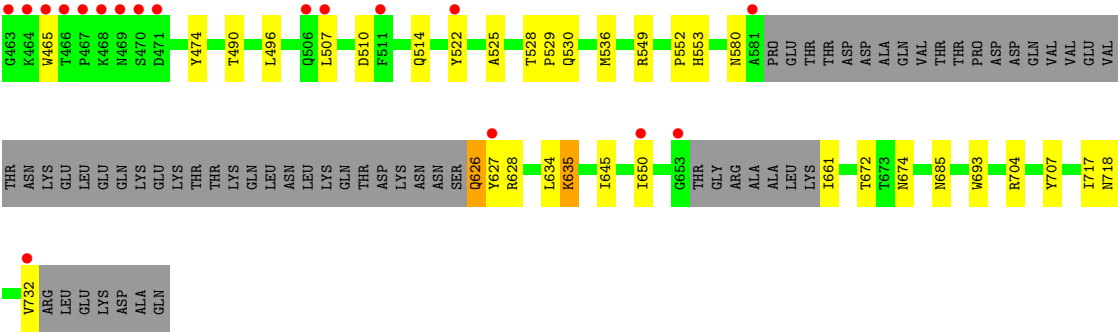
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			28	13	5	8	2		
2	B	1	Total	C	N	O	S	0	0
			28	13	5	8	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	127	Total	O	0	0
			127	127		
3	B	180	Total	O	0	0
			180	180		

- Molecule 1: Penicillin-binding protein 1a





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	119.08Å 242.57Å 49.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.94 – 2.60 47.94 – 2.60	Depositor EDS
% Data completeness (in resolution range)	92.6 (47.94-2.60) 92.6 (47.94-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.9.6	Depositor
R, R_{free}	0.191 , 0.241 0.192 , 0.238	Depositor DCC
R_{free} test set	2040 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 69.0	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	0.94	EDS
Total number of atoms	9762	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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

5.1 Standard geometry

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

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	0.83	0/4824	1.27	14/6541 (0.2%)
1	B	0.86	2/4793 (0.0%)	1.29	14/6501 (0.2%)
All	All	0.84	2/9617 (0.0%)	1.28	28/13042 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	672	THR	C-O	-5.25	1.17	1.23
1	B	248	MET	SD-CE	5.10	1.92	1.79

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	709	GLY	CA-C-N	8.25	136.56	121.70
1	A	709	GLY	C-N-CA	8.25	136.56	121.70
1	A	393	LYS	N-CA-C	-6.03	105.00	112.90
1	B	168	SER	N-CA-C	-5.95	101.71	110.52
1	A	685	ASN	CA-CB-CG	5.91	118.51	112.60
1	B	197	GLU	CA-C-N	5.89	128.46	120.38
1	B	197	GLU	C-N-CA	5.89	128.46	120.38
1	B	685	ASN	CA-CB-CG	5.87	118.47	112.60
1	B	157	ILE	N-CA-C	5.85	117.29	110.62
1	A	168	SER	N-CA-C	-5.82	101.91	110.52
1	B	296	GLY	N-CA-C	5.81	120.01	112.68
1	A	296	GLY	N-CA-C	5.68	119.83	112.68
1	B	628	ARG	N-CA-C	5.67	118.41	109.96
1	A	421	LYS	CA-C-N	5.67	130.41	121.56
1	A	421	LYS	C-N-CA	5.67	130.41	121.56
1	A	157	ILE	N-CA-C	5.67	117.08	110.62
1	A	645	ILE	N-CA-C	-5.57	105.29	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	439	PHE	CA-CB-CG	5.54	119.34	113.80
1	B	393	LYS	N-CA-C	-5.50	105.69	112.90
1	B	134	ASN	CA-C-N	5.43	127.50	120.44
1	B	134	ASN	C-N-CA	5.43	127.50	120.44
1	B	645	ILE	N-CA-C	-5.40	105.46	110.53
1	A	524	ILE	CA-C-N	5.37	128.02	120.28
1	A	524	ILE	C-N-CA	5.37	128.02	120.28
1	A	710	ILE	N-CA-CB	5.30	120.51	111.50
1	B	419	GLN	CB-CG-CD	-5.20	103.75	112.60
1	B	136	SER	N-CA-C	5.19	117.34	111.11
1	A	685	ASN	N-CA-C	-5.14	101.89	109.18

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	4715	0	4702	50	0
1	B	4684	0	4662	41	0
2	A	28	0	17	6	0
2	B	28	0	16	2	0
3	A	127	0	0	0	0
3	B	180	0	0	3	0
All	All	9762	0	9397	86	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 (86) 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:434:SER:CB	2:A:998:AZR:H20	1.76	1.13
1:A:298:ARG:H	1:A:390:GLN:HE22	1.12	0.95
1:B:298:ARG:H	1:B:390:GLN:HE22	1.10	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:SER:OG	2:A:998:AZR:H2O	0.76	0.93
1:A:434:SER:HG	2:A:998:AZR:H2O	1.22	0.90
1:B:431:GLN:HE21	1:B:528:THR:HA	1.37	0.89
1:A:431:GLN:HE21	1:A:528:THR:HA	1.40	0.85
1:A:549:ARG:NH1	1:A:550:VAL:O	2.15	0.79
1:A:135:LEU:HD12	1:A:135:LEU:H	1.48	0.78
1:A:313:TYR:CE1	1:A:419:GLN:HB2	2.19	0.77
1:B:435:THR:HG23	1:B:536:MET:HE2	1.68	0.75
1:B:356:ASN:ND2	1:B:704:ARG:H	1.88	0.71
1:B:434:SER:H	2:B:999:AZR:C2O	2.03	0.70
1:A:434:SER:CB	2:A:998:AZR:C2O	2.54	0.68
1:B:432:PRO:HB2	1:B:435:THR:HG22	1.79	0.65
1:A:71:PHE:O	1:B:553:HIS:HA	1.99	0.62
1:B:510:ASP:O	1:B:549:ARG:HD3	2.00	0.61
1:A:707:TYR:H	1:A:710:ILE:HG12	1.65	0.61
1:A:528:THR:N	1:A:529:PRO:HD2	2.16	0.60
1:B:528:THR:N	1:B:529:PRO:HD2	2.17	0.60
1:B:465:TRP:HZ3	1:B:522:TYR:HB2	1.67	0.58
1:B:446:GLU:OE2	1:B:635:LYS:HB2	2.04	0.58
1:B:406:GLY:O	1:B:552:PRO:HA	2.04	0.56
1:A:708:GLY:O	1:A:712:ALA:HB3	2.05	0.56
1:A:406:GLY:O	1:A:552:PRO:HA	2.05	0.55
1:A:396:GLY:O	1:A:414:GLY:HA2	2.08	0.53
1:B:435:THR:CG2	1:B:536:MET:HE2	2.39	0.53
1:A:137:LYS:NZ	1:B:256:HIS:HD2	2.08	0.52
1:A:380:ASN:ND2	1:A:385:ALA:H	2.07	0.51
1:B:418:TYR:HB2	3:B:873:HOH:O	2.10	0.51
1:A:707:TYR:O	1:A:709:GLY:HA3	2.10	0.50
1:B:37:GLN:HB2	3:B:889:HOH:O	2.10	0.50
1:B:191:ASN:HB3	1:B:194:VAL:HG12	1.93	0.49
1:A:66:ALA:HA	1:A:206:ILE:HG12	1.94	0.49
1:A:553:HIS:HA	1:B:71:PHE:O	2.12	0.49
1:A:323:LYS:HE2	1:A:325:ASN:HD21	1.77	0.49
1:B:356:ASN:HD22	1:B:704:ARG:H	1.59	0.49
1:B:179:MET:HE2	1:B:203:ARG:HD3	1.95	0.48
1:B:707:TYR:N	1:B:707:TYR:CD2	2.82	0.48
1:A:179:MET:HE2	1:A:203:ARG:HD3	1.96	0.48
1:B:434:SER:N	2:B:999:AZR:C2O	2.76	0.47
1:B:381:GLU:H	1:B:381:GLU:CD	2.22	0.47
1:A:51:GLU:HB2	1:A:54:GLN:HG3	1.96	0.47
1:A:496:LEU:HD22	1:A:525:ALA:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:VAL:HB	1:A:40:ALA:HB3	1.95	0.46
1:A:69:SER:HB3	3:B:857:HOH:O	2.16	0.46
1:B:323:LYS:HE3	1:B:325:ASN:HD21	1.81	0.45
1:A:432:PRO:HD2	1:A:527:GLY:O	2.15	0.45
1:A:397:GLN:HG3	1:A:693:TRP:HB3	1.99	0.45
1:B:496:LEU:HD22	1:B:525:ALA:HB2	1.97	0.45
1:A:431:GLN:NE2	1:A:528:THR:HA	2.21	0.45
1:B:474:TYR:HE1	1:B:490:THR:HG21	1.81	0.45
1:A:166:ASN:HB2	1:A:234:PRO:HD3	2.00	0.44
1:B:350:ARG:HH11	1:B:358:VAL:HG21	1.82	0.44
1:A:474:TYR:HE1	1:A:490:THR:HG21	1.83	0.44
1:A:514:GLN:HB3	1:A:517:GLN:HG2	1.99	0.44
1:B:397:GLN:HG3	1:B:693:TRP:HB3	1.98	0.44
1:A:640:TYR:HD1	1:A:732:VAL:HG23	1.82	0.44
1:A:135:LEU:H	1:A:135:LEU:CD1	2.24	0.44
1:A:247:GLU:HG2	1:A:417:PHE:HE1	1.81	0.44
1:A:509:MET:HE3	1:A:515:GLU:HB2	2.00	0.43
1:A:255:LYS:HG3	1:B:185:LYS:HE3	2.00	0.43
1:A:29:LEU:HD22	1:A:266:TYR:O	2.18	0.43
1:B:626:GLN:N	1:B:626:GLN:OE1	2.52	0.43
1:B:66:ALA:HA	1:B:206:ILE:HG12	2.01	0.43
1:A:72:PHE:O	1:B:553:HIS:HB2	2.19	0.42
1:B:661:ILE:HD11	1:B:717:ILE:HA	2.01	0.42
1:A:350:ARG:HH11	1:A:358:VAL:HG21	1.84	0.42
1:B:528:THR:H	1:B:529:PRO:HD2	1.85	0.42
1:A:511:PHE:HA	1:A:549:ARG:HD3	2.02	0.42
1:B:221:TYR:O	1:B:225:VAL:HG22	2.20	0.42
1:B:707:TYR:N	1:B:707:TYR:HD2	2.17	0.42
1:A:221:TYR:O	1:A:225:VAL:HG22	2.20	0.41
1:B:431:GLN:NE2	1:B:528:THR:HA	2.19	0.41
1:A:519:PRO:HD2	1:A:524:ILE:HG22	2.02	0.41
1:A:298:ARG:H	1:A:390:GLN:NE2	1.96	0.41
1:A:434:SER:HB2	2:A:998:AZR:C20	2.44	0.41
1:A:29:LEU:HB3	1:A:42:TYR:HB2	2.03	0.41
1:B:432:PRO:HD3	1:B:529:PRO:O	2.20	0.41
1:A:626:GLN:HA	1:A:627:TYR:HA	1.84	0.41
1:A:674:ASN:N	2:A:998:AZR:N15	2.69	0.41
1:B:166:ASN:HB2	1:B:234:PRO:HD3	2.02	0.41
1:B:29:LEU:HB3	1:B:42:TYR:HB2	2.03	0.41
1:B:443:LEU:O	1:B:446:GLU:HB2	2.20	0.41
1:A:380:ASN:HD21	1:A:385:ALA:H	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:GLU:HG2	1:A:417:PHE:CE1	2.55	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	590/731 (81%)	557 (94%)	27 (5%)	6 (1%)	12	28
1	B	587/731 (80%)	562 (96%)	23 (4%)	2 (0%)	36	58
All	All	1177/1462 (80%)	1119 (95%)	50 (4%)	8 (1%)	18	38

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	383	LYS
1	A	708	GLY
1	B	627	TYR
1	A	349	ALA
1	B	349	ALA
1	A	384	THR
1	A	463	GLY
1	A	709	GLY

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	490/608 (81%)	468 (96%)	22 (4%)	24	50
1	B	486/608 (80%)	471 (97%)	15 (3%)	35	63
All	All	976/1216 (80%)	939 (96%)	37 (4%)	29	56

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
1	A	39	ILE
1	A	135	LEU
1	A	139	ASP
1	A	145	VAL
1	A	198	ARG
1	A	259	GLU
1	A	353	ARG
1	A	381	GLU
1	A	384	THR
1	A	421	LYS
1	A	462	ILE
1	A	514	GLN
1	A	518	ILE
1	A	530	GLN
1	A	568	GLU
1	A	650	ILE
1	A	674	ASN
1	A	698	GLN
1	A	710	ILE
1	A	718	ASN
1	A	732	VAL
1	B	35	ASP
1	B	145	VAL
1	B	259	GLU
1	B	435	THR
1	B	507	LEU
1	B	514	GLN
1	B	530	GLN
1	B	580	ASN
1	B	626	GLN
1	B	634	LEU
1	B	635	LYS
1	B	650	ILE
1	B	674	ASN

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Mol	Chain	Res	Type
1	B	718	ASN
1	B	732	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	61	HIS
1	A	153	ASN
1	A	195	ASN
1	A	212	GLN
1	A	256	HIS
1	A	260	GLN
1	A	285	GLN
1	A	295	HIS
1	A	325	ASN
1	A	380	ASN
1	A	390	GLN
1	A	431	GLN
1	A	497	GLN
1	A	514	GLN
1	A	556	GLN
1	A	629	GLN
1	A	652	HIS
1	A	722	GLN
1	B	37	GLN
1	B	61	HIS
1	B	153	ASN
1	B	166	ASN
1	B	256	HIS
1	B	260	GLN
1	B	285	GLN
1	B	325	ASN
1	B	356	ASN
1	B	390	GLN
1	B	431	GLN
1	B	497	GLN
1	B	514	GLN
1	B	551	GLN
1	B	629	GLN
1	B	674	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	AZR	B	999	1	26,28,28	2.42	8 (30%)	31,41,41	1.87	9 (29%)
2	AZR	A	998	1	26,28,28	2.24	5 (19%)	31,41,41	1.93	11 (35%)

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	AZR	B	999	1	-	6/32/35/35	0/1/1/1
2	AZR	A	998	1	-	6/32/35/35	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	998	AZR	S17-N12	9.64	1.71	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	999	AZR	S17-N12	9.51	1.71	1.59
2	B	999	AZR	O11-N14	-3.59	1.34	1.42
2	B	999	AZR	O32-S17	3.36	1.45	1.42
2	A	998	AZR	O32-S17	2.79	1.45	1.42
2	B	999	AZR	O34-S17	2.69	1.45	1.42
2	B	999	AZR	C19-C18	-2.56	1.51	1.54
2	B	999	AZR	C26-S8	-2.54	1.71	1.74
2	A	998	AZR	C26-S8	-2.18	1.71	1.74
2	A	998	AZR	O34-S17	2.14	1.44	1.42
2	B	999	AZR	C19-N13	-2.13	1.43	1.46
2	B	999	AZR	C22-C24	-2.05	1.43	1.46
2	A	998	AZR	C19-C18	-2.04	1.52	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	999	AZR	O32-S17-N12	-4.84	100.79	108.88
2	B	999	AZR	C25-S8-C26	3.75	90.46	88.84
2	A	998	AZR	O10-C21-N13	3.74	129.68	123.09
2	A	998	AZR	C20-C19-N13	-3.54	104.22	109.80
2	A	998	AZR	C23-O11-N14	3.35	113.30	110.35
2	B	999	AZR	O10-C21-N13	3.32	128.94	123.09
2	A	998	AZR	O32-S17-O34	-3.15	113.36	120.36
2	A	998	AZR	C27-C23-C29	-3.12	98.63	110.00
2	A	998	AZR	O11-C23-C29	2.98	114.20	109.66
2	B	999	AZR	O11-C23-C29	2.84	113.98	109.66
2	A	998	AZR	N16-C26-N15	2.45	126.90	124.05
2	B	999	AZR	O10-C21-C22	-2.39	117.76	121.60
2	B	999	AZR	C27-C23-C29	-2.35	101.44	110.00
2	B	999	AZR	O32-S17-O34	-2.33	115.17	120.36
2	A	998	AZR	O11-N14-C22	2.33	115.39	111.76
2	B	999	AZR	N16-C26-N15	2.31	126.73	124.05
2	A	998	AZR	C25-S8-C26	2.22	89.80	88.84
2	B	999	AZR	C20-C19-N13	-2.09	106.50	109.80
2	A	998	AZR	C7-C18-N12	-2.08	106.82	110.45
2	A	998	AZR	C22-C21-N13	-2.02	111.09	114.27

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	999	AZR	C18-C19-C20-O9

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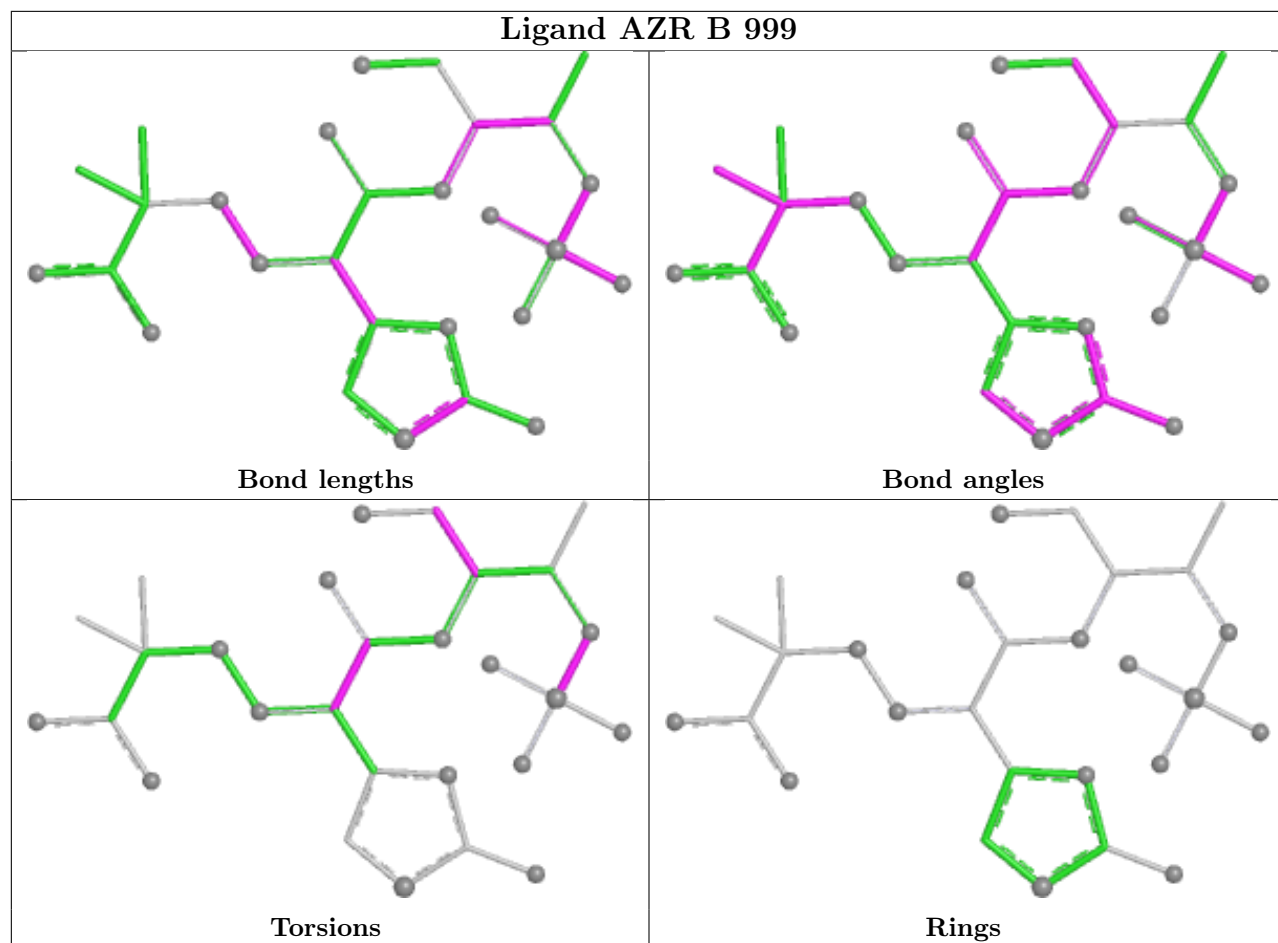
Mol	Chain	Res	Type	Atoms
2	A	998	AZR	O10-C21-C22-C24
2	A	998	AZR	N13-C21-C22-C24
2	B	999	AZR	O10-C21-C22-C24
2	A	998	AZR	O10-C21-C22-N14
2	B	999	AZR	N13-C21-C22-C24
2	A	998	AZR	C18-N12-S17-O34
2	A	998	AZR	C18-C19-C20-O9
2	A	998	AZR	N13-C21-C22-N14
2	B	999	AZR	N13-C21-C22-N14
2	B	999	AZR	O10-C21-C22-N14
2	B	999	AZR	C18-N12-S17-O34

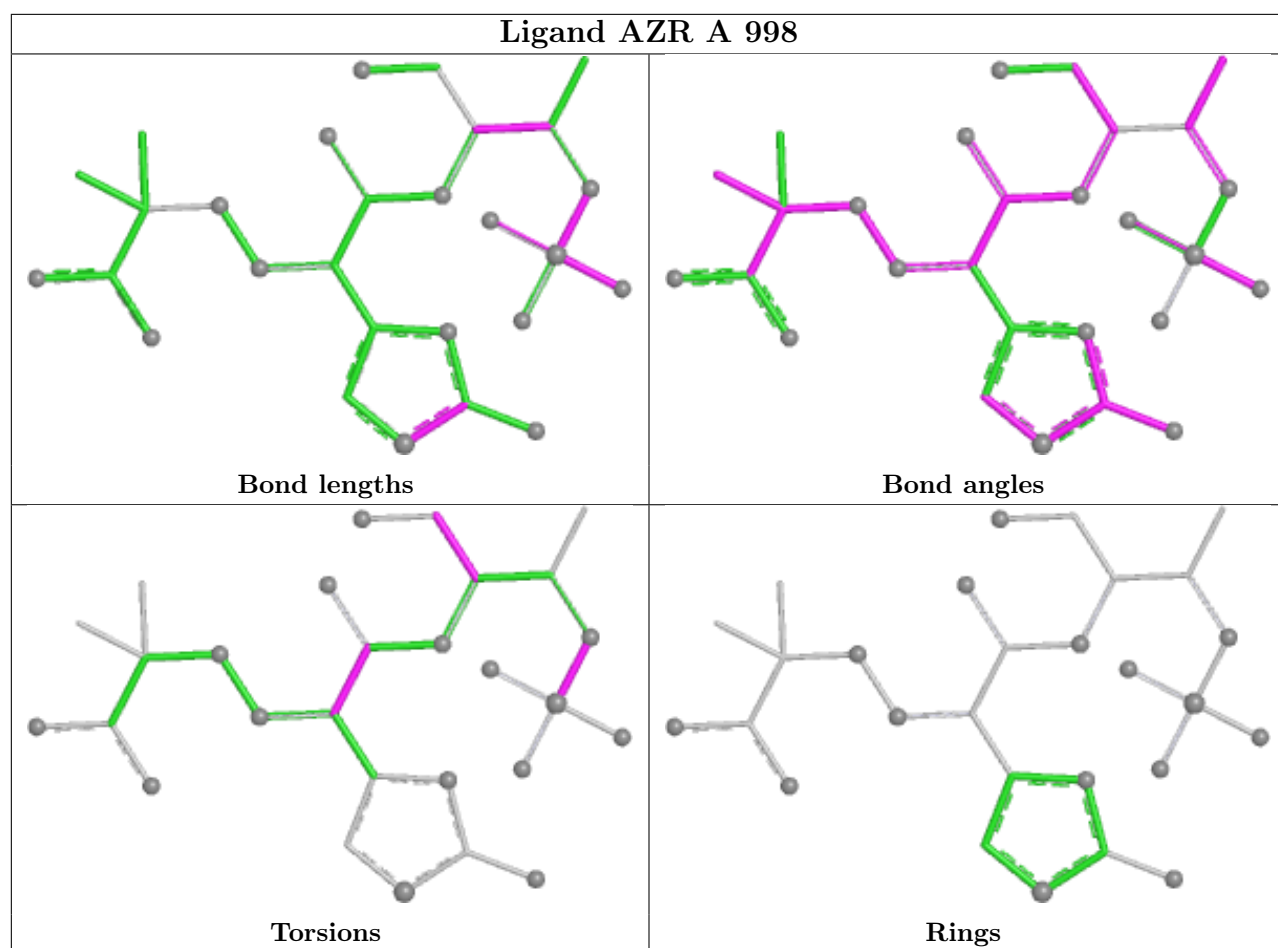
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	999	AZR	2	0
2	A	998	AZR	6	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.





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	598/731 (81%)	0.23	18 (3%)	52 47	23, 54, 97, 123	0
1	B	595/731 (81%)	-0.03	26 (4%)	39 33	15, 44, 93, 143	0
All	All	1193/1462 (81%)	0.10	44 (3%)	45 39	15, 49, 95, 143	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	460	ILE	4.5
1	B	581	ALA	4.3
1	B	459	PRO	4.2
1	B	511	PHE	4.2
1	B	465	TRP	3.9
1	B	732	VAL	3.4
1	B	653	GLY	3.4
1	A	654	THR	3.4
1	B	627	TYR	3.4
1	A	736	LYS	3.3
1	B	469	ASN	3.3
1	B	507	LEU	3.3
1	A	709	GLY	3.1
1	A	383	LYS	3.0
1	A	511	PHE	3.0
1	A	562	TYR	3.0
1	B	466	THR	3.0
1	B	468	LYS	2.9
1	B	470	SER	2.9
1	B	458	SER	2.8
1	B	522	TYR	2.7
1	B	194	VAL	2.6
1	B	463	GLY	2.5
1	A	360	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	133	GLN	2.5
1	B	462	ILE	2.5
1	B	506	GLN	2.5
1	A	134	ASN	2.4
1	A	708	GLY	2.3
1	B	228	PRO	2.3
1	B	471	ASP	2.3
1	A	733	ARG	2.3
1	B	464	LYS	2.2
1	A	707	TYR	2.2
1	B	467	PRO	2.2
1	A	561	ALA	2.2
1	B	53	LYS	2.2
1	B	650	ILE	2.2
1	A	472	GLY	2.1
1	A	447	ARG	2.1
1	A	135	LEU	2.1
1	A	362	PRO	2.1
1	A	324	VAL	2.1
1	A	734	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](#)

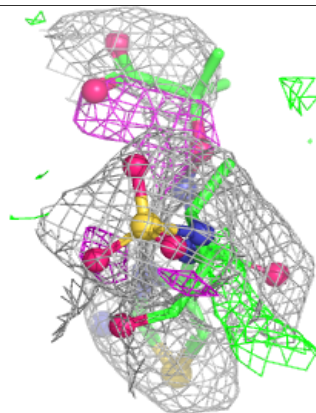
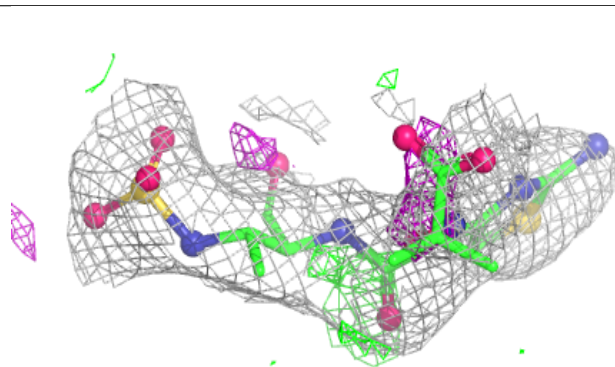
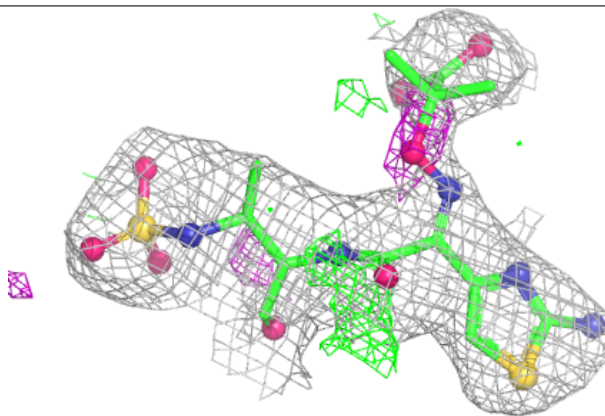
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

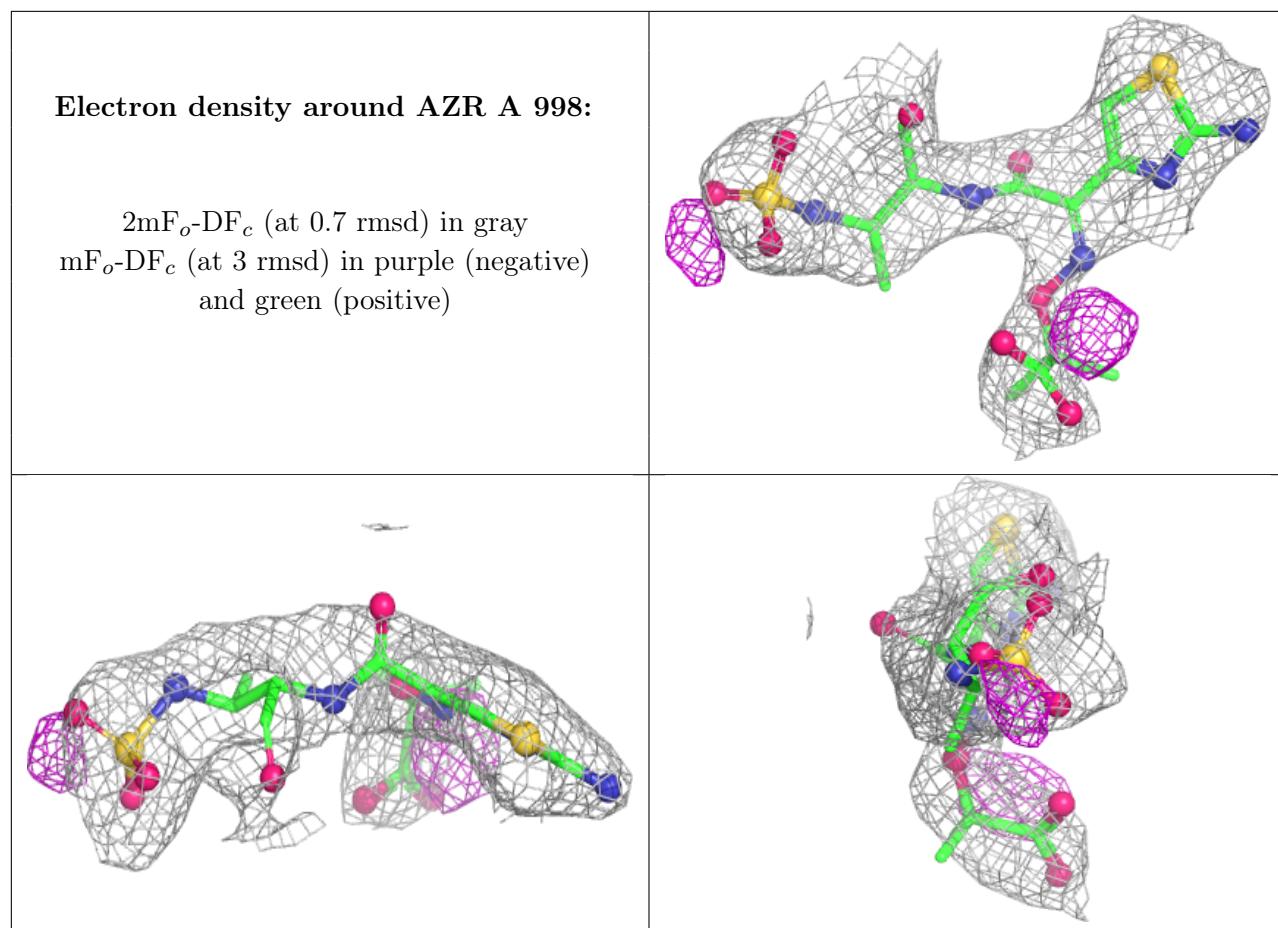
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	AZR	B	999	28/28	0.85	0.15	54,65,92,96	0
2	AZR	A	998	28/28	0.86	0.14	61,80,93,93	0

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 AZR B 999:

$2mF_o-DF_c$ (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.