Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:52 PM GMT

PDB ID	:	1VM1
Title	:	STRUCTURE OF SHV-1 BETA-LACTAMASE INHIBITED BY TAZOBACTAM
Authors	:	Kuzin, A.P.; Nukaga, M.; Nukaga, Y.; Hujer, A.; Bonomo, R.A.; Knox, J.R.
Deposited on	:	2004-08-27
Resolution	:	2.02 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 (i) symbol.

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

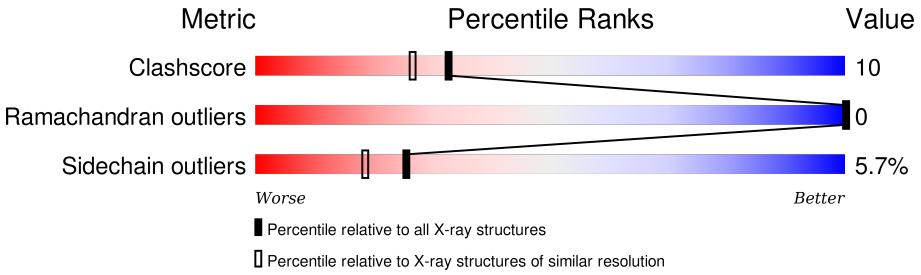
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 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))
Clashscore	102246	9060 (2.04-2.00)
Ramachandran outliers	100387	8952 (2.04-2.00)
Sidechain outliers	100360	8951 (2.04-2.00)

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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	265	68% 26% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MA4	A	300	X	-	-	-
5	TAZ	A	504	X	-	-	-

2 Entry composition

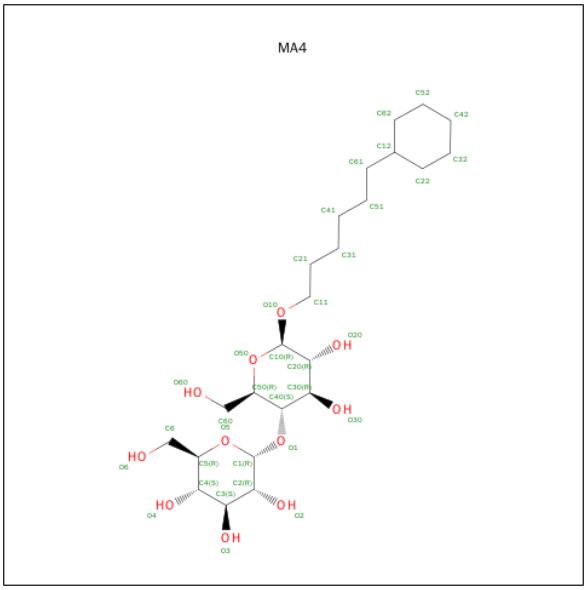
There are 6 unique types of molecules in this entry. The entry contains 2285 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BETA-LACTAMASE SHV-1.

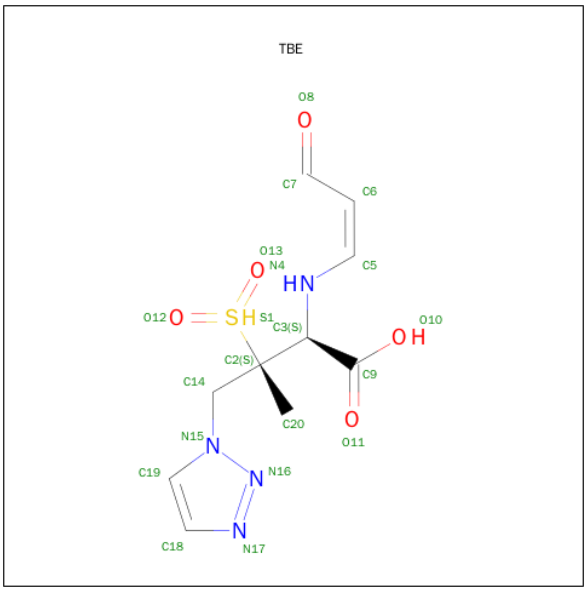
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	265	2023	1256	373	383	11	0	0	0

- Molecule 2 is CYCLOHEXYL-HEXYL-BETA-D-MALTOSIDE (three-letter code: MA4) (formula: $C_{24}H_{44}O_{11}$).



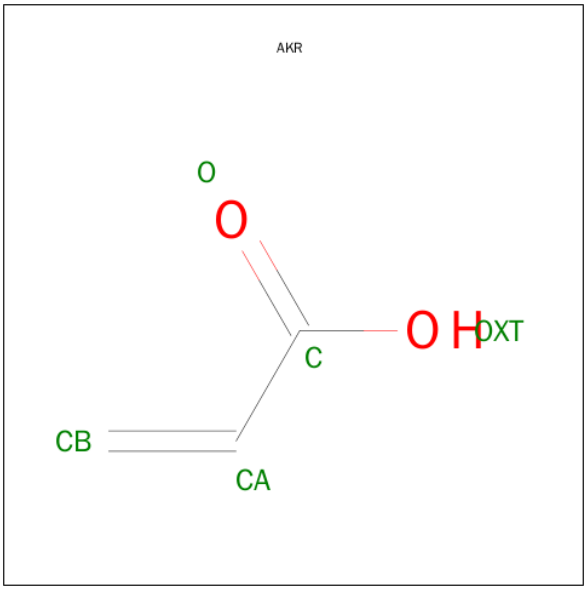
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	35	24	11	0	0
			Total	C			
2	A	1	7	7		0	0

- Molecule 3 is TAZOBACTAM INTERMEDIATE (three-letter code: TBE) (formula: $C_{10}H_{14}N_4O_5S$).



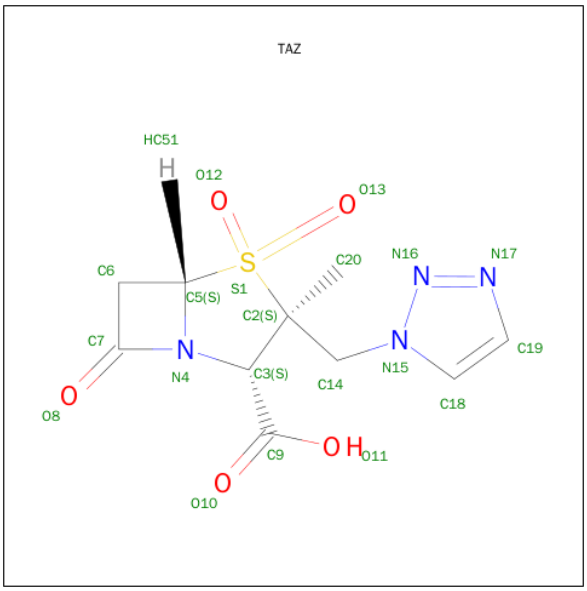
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			20	10	4	5	1		

- Molecule 4 is ACRYLIC ACID (three-letter code: AKR) (formula: $C_3H_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			5	3	2			

- Molecule 5 is TAZOBACTAM (three-letter code: TAZ) (formula: $C_{10}H_{12}N_4O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			20	10	4	5	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	175	Total	O	0	0
			175	175		

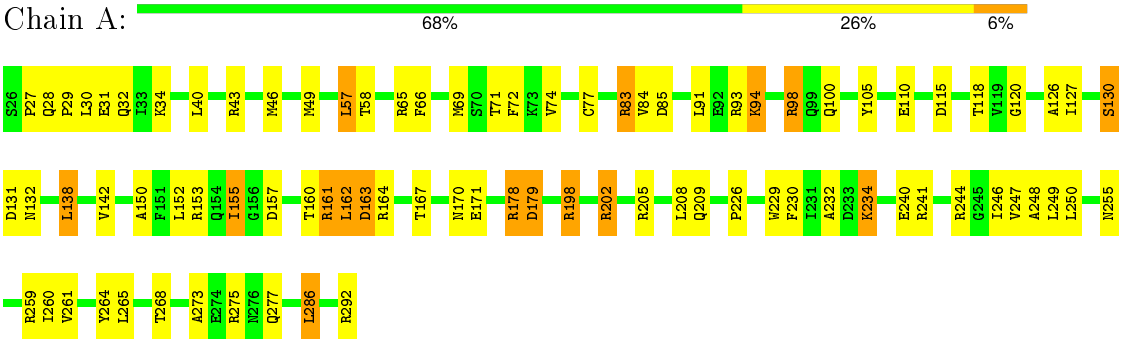
3 Residue-property plots (i)

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.

Note EDS was not executed.

- Molecule 1: BETA-LACTAMASE SHV-1

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	49.20Å 56.10Å 82.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.02	Depositor
% Data completeness (in resolution range)	95.0 (50.00-2.02)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.171 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2285	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AKR, TBE, MA4, TAZ

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	0.81	0/2053	1.86	53/2781 (1.9%)

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	34	LYS	CB-CG-CD	15.82	152.74	111.60
1	A	244	ARG	CD-NE-CZ	14.50	143.90	123.60
1	A	93	ARG	NE-CZ-NH1	-14.43	113.08	120.30
1	A	83	ARG	NE-CZ-NH2	-11.25	114.67	120.30
1	A	65	ARG	NE-CZ-NH1	11.17	125.89	120.30
1	A	161	ARG	NE-CZ-NH1	10.94	125.77	120.30
1	A	292	ARG	NE-CZ-NH2	10.14	125.37	120.30
1	A	153	ARG	NE-CZ-NH2	9.95	125.28	120.30
1	A	178	ARG	NE-CZ-NH1	9.41	125.01	120.30
1	A	65	ARG	CD-NE-CZ	9.02	136.22	123.60
1	A	85	ASP	CB-CG-OD1	8.89	126.31	118.30
1	A	83	ARG	NE-CZ-NH1	8.51	124.55	120.30
1	A	202	ARG	NE-CZ-NH2	8.26	124.43	120.30
1	A	292	ARG	CA-C-O	-8.16	102.96	120.10
1	A	264	TYR	CB-CG-CD1	7.95	125.77	121.00
1	A	65	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	A	198	ARG	NE-CZ-NH1	-7.80	116.40	120.30
1	A	265	LEU	CA-CB-CG	7.76	133.16	115.30
1	A	264	TYR	CB-CG-CD2	-7.63	116.42	121.00
1	A	83	ARG	CD-NE-CZ	7.55	134.17	123.60
1	A	205	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	A	138	LEU	CA-CB-CG	7.33	132.15	115.30
1	A	275	ARG	NE-CZ-NH1	-7.17	116.72	120.30
1	A	244	ARG	NE-CZ-NH2	7.12	123.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	244	ARG	NE-CZ-NH1	-7.09	116.75	120.30
1	A	98	ARG	NE-CZ-NH1	-6.87	116.86	120.30
1	A	72	PHE	CB-CG-CD2	6.63	125.44	120.80
1	A	153	ARG	NE-CZ-NH1	-6.63	116.98	120.30
1	A	105	TYR	CB-CG-CD1	-6.55	117.07	121.00
1	A	275	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	A	275	ARG	NH1-CZ-NH2	6.10	126.11	119.40
1	A	66	PHE	CB-CG-CD2	6.01	125.01	120.80
1	A	161	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	A	93	ARG	NE-CZ-NH2	5.91	123.26	120.30
1	A	234	LYS	CG-CD-CE	5.85	129.44	111.90
1	A	247	VAL	CG1-CB-CG2	-5.83	101.58	110.90
1	A	72	PHE	CB-CG-CD1	-5.71	116.81	120.80
1	A	43	ARG	CD-NE-CZ	5.64	131.50	123.60
1	A	292	ARG	NH1-CZ-NH2	-5.57	113.27	119.40
1	A	163	ASP	CB-CG-OD2	-5.50	113.34	118.30
1	A	248	ALA	CB-CA-C	-5.49	101.86	110.10
1	A	150	ALA	O-C-N	-5.45	113.98	122.70
1	A	205	ARG	NH1-CZ-NH2	5.45	125.39	119.40
1	A	131	ASP	CB-CG-OD2	-5.41	113.44	118.30
1	A	115	ASP	CB-CG-OD2	-5.39	113.44	118.30
1	A	46	MET	CA-CB-CG	5.31	122.33	113.30
1	A	255	ASN	CB-CG-OD1	-5.30	111.01	121.60
1	A	157	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	179	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	A	105	TYR	CA-CB-CG	-5.12	103.66	113.40
1	A	244	ARG	CG-CD-NE	5.10	122.51	111.80
1	A	240	GLU	OE1-CD-OE2	-5.07	117.22	123.30
1	A	40	LEU	CB-CA-C	-5.04	100.62	110.20

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	2023	0	2043	40	0
2	A	42	0	51	5	0
3	A	20	0	12	5	0
4	A	5	0	2	0	0
5	A	20	0	11	1	0
6	A	175	0	0	4	0
All	All	2285	0	2119	44	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 10.

All (44) 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)
2:A:300:MA4:H111	2:A:300:MA4:O20	1.67	0.93
3:A:501:TBE:O13	3:A:501:TBE:N4	2.20	0.75
1:A:74:VAL:HG23	1:A:234:LYS:HG2	1.68	0.73
1:A:29:PRO:HB3	1:A:286:LEU:HD13	1.75	0.68
2:A:300:MA4:O20	2:A:300:MA4:C11	2.40	0.67
3:A:501:TBE:H3	3:A:501:TBE:C19	2.28	0.64
1:A:273:ALA:O	1:A:277:GLN:HG3	2.03	0.59
1:A:226:PRO:HB3	2:A:300:MA4:H31	1.84	0.59
1:A:132:ASN:ND2	3:A:501:TBE:O12	2.35	0.59
1:A:170:ASN:OD1	3:A:501:TBE:H19	2.04	0.57
1:A:49:MET:CE	1:A:260:ILE:HD12	2.36	0.55
1:A:28:GLN:HB2	1:A:31:GLU:OE1	2.07	0.54
1:A:261:VAL:HG11	2:A:300:MA4:H321	1.89	0.54
1:A:69:MET:HA	1:A:170:ASN:HD22	1.74	0.53
1:A:83:ARG:HD2	1:A:142:VAL:HG12	1.91	0.53
1:A:161:ARG:HH21	1:A:163:ASP:CG	2.13	0.52
1:A:71:THR:HA	1:A:234:LYS:HG3	1.92	0.51
1:A:167:THR:HB	3:A:501:TBE:C19	2.40	0.51
1:A:246:ILE:HD13	2:A:300:MA4:H121	1.92	0.51
1:A:29:PRO:HG2	6:A:754:HOH:O	2.10	0.51
1:A:57:LEU:HD13	1:A:259:ARG:HD3	1.93	0.51
1:A:58:THR:HG23	6:A:730:HOH:O	2.11	0.50
1:A:209:GLN:NE2	6:A:635:HOH:O	2.41	0.50
1:A:171:GLU:O	1:A:241:ARG:NH1	2.44	0.50
1:A:164:ARG:NH2	1:A:171:GLU:OE2	2.44	0.49
1:A:84:VAL:HG21	1:A:91:LEU:HD22	1.96	0.48
1:A:27:PRO:HG2	1:A:32:GLN:HB2	1.96	0.48
1:A:84:VAL:HG21	1:A:91:LEU:CD2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LEU:HD23	1:A:160:THR:HB	1.97	0.47
1:A:77:CYS:HB2	1:A:127:ILE:HD11	1.96	0.47
1:A:202:ARG:HD3	6:A:682:HOH:O	2.15	0.47
1:A:162:LEU:HD22	1:A:179:ASP:OD2	2.16	0.45
1:A:226:PRO:HG2	1:A:229:TRP:CD1	2.52	0.45
1:A:155:ILE:HG13	1:A:198:ARG:NE	2.33	0.43
1:A:232:ALA:HB3	1:A:249:LEU:HB2	2.01	0.43
1:A:126:ALA:O	1:A:130:SER:HA	2.19	0.43
1:A:91:LEU:HD12	1:A:120:GLY:HA2	2.00	0.43
1:A:110:GLU:OE2	5:A:504:TAZ:O10	2.36	0.42
1:A:74:VAL:CG2	1:A:234:LYS:HG2	2.45	0.41
1:A:94:LYS:HA	1:A:118:THR:HA	2.01	0.41
1:A:69:MET:HA	1:A:170:ASN:ND2	2.35	0.41
1:A:161:ARG:NH2	1:A:178:ARG:HG2	2.35	0.40
1:A:57:LEU:HD22	1:A:259:ARG:NH1	2.36	0.40
1:A:230:PHE:O	1:A:250:LEU:HD12	2.22	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	263/265 (99%)	258 (98%)	5 (2%)	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	211/211 (100%)	199 (94%)	12 (6%)	25 18

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	57	LEU
1	A	94	LYS
1	A	98	ARG
1	A	100	GLN
1	A	130	SER
1	A	138	LEU
1	A	155	ILE
1	A	162	LEU
1	A	208	LEU
1	A	268	THR
1	A	286	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	32	GLN
1	A	112	HIS
1	A	197	GLN
1	A	209	GLN
1	A	289	HIS

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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

5 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	MA4	A	300	-	37,37,37	2.12	8 (21%)	50,50,50	2.51	21 (42%)
2	MA4	A	301	-	7,7,37	0.54	0	8,8,50	2.57	4 (50%)
3	TBE	A	501	1	12,20,20	3.11	4 (33%)	6,27,27	2.05	2 (33%)
4	AKR	A	503	1	1,4,4	0.23	0	0,4,4	0.00	-
5	TAZ	A	504	-	15,22,22	1.28	2 (13%)	14,36,36	2.48	5 (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	MA4	A	300	-	2/2/11/11	0/18/66/66	0/3/3/3
2	MA4	A	301	-	-	0/0/8/66	0/1/1/3
3	TBE	A	501	1	-	1/12/26/26	0/1/1/1
4	AKR	A	503	1	-	0/0/2/2	0/0/0/0
5	TAZ	A	504	-	1/1/7/7	0/3/46/46	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	MA4	C4-C5	-5.54	1.41	1.53
2	A	300	MA4	C30-C20	-5.19	1.38	1.52
2	A	300	MA4	C10-C20	-4.73	1.38	1.52
2	A	300	MA4	C40-C50	-4.36	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	MA4	C4-C3	-4.15	1.41	1.52
2	A	300	MA4	C3-C2	-3.91	1.42	1.52
2	A	300	MA4	C1-C2	-3.66	1.41	1.52
2	A	300	MA4	C30-C40	-3.36	1.42	1.52
5	A	504	TAZ	N17-N16	-2.38	1.31	1.34
3	A	501	TBE	C2-S1	-2.36	1.76	1.85
3	A	501	TBE	N17-N16	-2.16	1.31	1.34
5	A	504	TAZ	C14-C2	2.39	1.55	1.53
3	A	501	TBE	C6-C7	2.81	1.52	1.44
3	A	501	TBE	C5-C6	9.54	1.52	1.37

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	300	MA4	C61-C12-C22	-6.04	99.30	112.10
2	A	301	MA4	C61-C12-C22	-5.19	100.17	112.12
2	A	300	MA4	C61-C12-C62	-5.15	101.18	112.10
5	A	504	TAZ	O8-C7-N4	-4.36	122.48	130.21
3	A	501	TBE	C19-N15-N16	-3.95	108.68	111.41
2	A	300	MA4	C42-C32-C22	-3.37	104.37	111.44
2	A	300	MA4	C52-C62-C12	-3.23	107.01	112.22
2	A	301	MA4	C61-C12-C62	-2.90	105.43	112.12
2	A	300	MA4	O2-C2-C3	-2.81	104.02	110.34
3	A	501	TBE	C14-C2-S1	-2.60	97.59	107.16
5	A	504	TAZ	C3-N4-C7	-2.35	122.23	127.14
2	A	300	MA4	C32-C22-C12	-2.17	108.72	112.22
2	A	301	MA4	C62-C12-C22	2.01	115.02	109.86
2	A	300	MA4	O5-C5-C4	2.05	113.52	109.68
2	A	300	MA4	O20-C20-C30	2.13	115.14	110.34
2	A	300	MA4	O50-C50-C60	2.19	111.89	106.36
2	A	300	MA4	O30-C30-C20	2.23	115.35	110.34
2	A	300	MA4	O50-C10-C20	2.58	115.56	110.28
5	A	504	TAZ	O13-S1-O12	2.65	122.59	118.96
2	A	300	MA4	C6-C5-C4	2.79	119.90	113.02
2	A	301	MA4	C42-C52-C62	3.22	118.18	111.44
2	A	300	MA4	C30-C40-C50	3.35	118.41	110.84
5	A	504	TAZ	O12-S1-C2	3.38	118.02	109.94
2	A	300	MA4	O50-C50-C40	3.41	116.94	109.75
2	A	300	MA4	C3-C4-C5	3.71	116.67	110.20
2	A	300	MA4	C1-C2-C3	3.73	117.33	109.97
2	A	300	MA4	C10-O50-C50	3.76	121.04	113.75
2	A	300	MA4	C20-C30-C40	4.02	118.42	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	300	MA4	C60-C50-C40	4.52	126.41	113.25
2	A	300	MA4	C10-C20-C30	5.25	120.32	109.97
2	A	300	MA4	O10-C10-C20	5.54	115.04	108.04
5	A	504	TAZ	O8-C7-C6	5.55	142.78	136.78

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	300	MA4	C2
2	A	300	MA4	C30
5	A	504	TAZ	C5

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	TBE	O8-C7-C6-C5

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	MA4	5	0
3	A	501	TBE	5	0
5	A	504	TAZ	1	0

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

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.