WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 09:11 AM EST

PDB ID	:	1B90
Title	:	BACILLUS CEREUS BETA-AMYLASE APO FORM
Authors	:	Mikami, B.; Adachi, M.; Kage, T.; Sarikaya, E.; Nanmori, T.; Shinke, R.; Utsumi, S.
Deposited on	:	1999-03-06
Resolution	:	2.50 Å(reported)

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

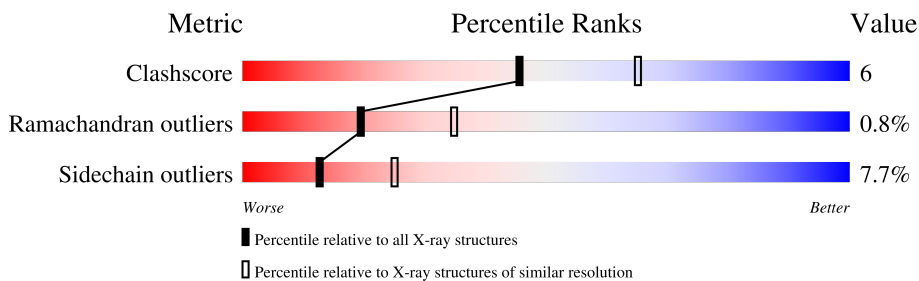|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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	Percentile Ranks	Value
Clashscore		6
Ramachandran outliers		0.8%
Sidechain outliers		7.7%

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 <=5%

Note EDS was not executed.

| Mol	Chain	Length	Quality of chain
1	A	516	75% 22% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4249 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 PROTEIN (BETA-AMYLASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total 4119	C 2645	N 676	O 781	S 17	0	0	0

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).
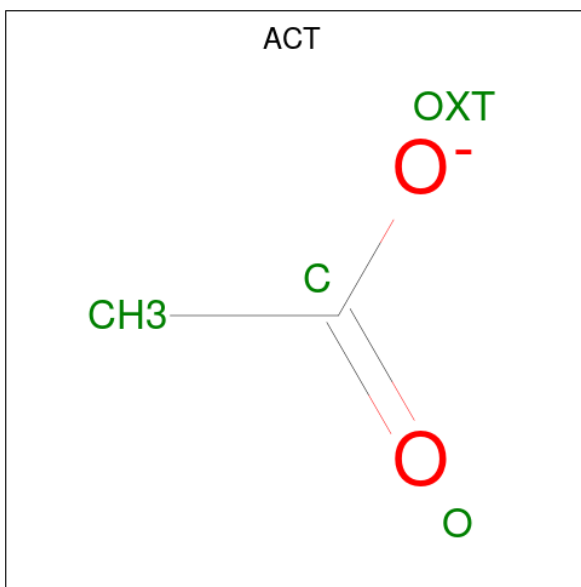
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1

O

O3 O⁻ —— S —— O⁻ O4

S

O

O2

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Ca 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	120	Total 120	O 120	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. 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. 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: PROTEIN (BETA-AMYLASE)
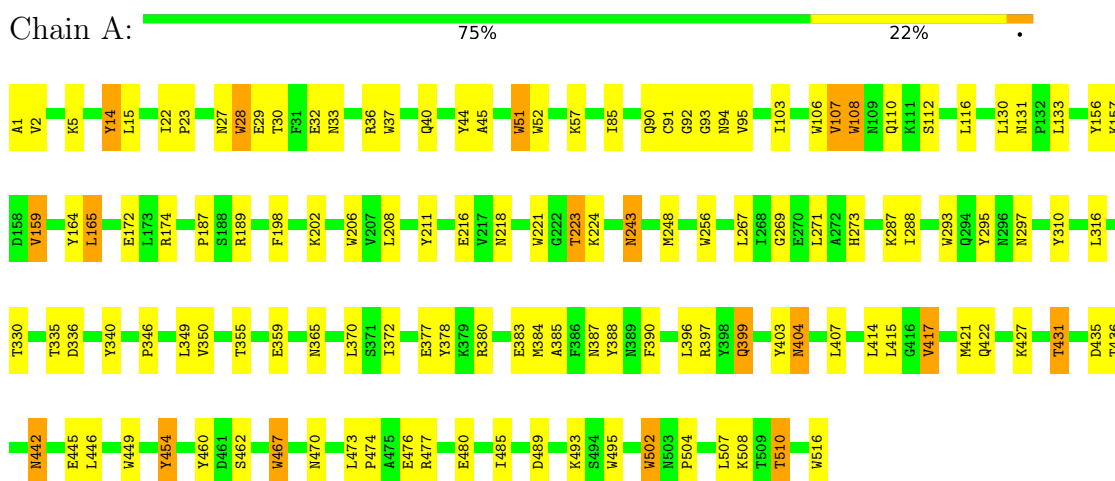
4 Data and refinement statistics ⓘ

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	57.08Å 92.10Å 65.67Å 90.00° 101.81° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	84.7 (10.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.164 , 0.247	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4249	wwPDB-VP
Average B, all atoms (Å^2)	19.0	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: ACT, SO4, CA

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	0.85	0/4234	1.57	71/5751 (1.2%)

There are no bond length outliers.

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	37	TRP	CD1-CG-CD2	9.21	113.67	106.30
1	A	28	TRP	CD1-CG-CD2	9.16	113.63	106.30
1	A	495	TRP	CD1-CG-CD2	8.70	113.26	106.30
1	A	37	TRP	CE2-CD2-CG	-8.64	100.39	107.30
1	A	189	ARG	NE-CZ-NH1	8.61	124.60	120.30
1	A	106	TRP	CD1-CG-CD2	8.30	112.94	106.30
1	A	516	TRP	CD1-CG-CD2	8.22	112.87	106.30
1	A	502	TRP	CD1-CG-CD2	8.17	112.83	106.30
1	A	206	TRP	CD1-CG-CD2	8.16	112.83	106.30
1	A	340	TYR	CB-CG-CD1	-8.14	116.11	121.00
1	A	477	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	A	403	TYR	CB-CG-CD2	-8.12	116.13	121.00
1	A	449	TRP	CD1-CG-CD2	8.09	112.77	106.30
1	A	51	TRP	CD1-CG-CD2	8.07	112.76	106.30
1	A	28	TRP	CE2-CD2-CG	-8.06	100.85	107.30
1	A	108	TRP	CD1-CG-CD2	8.04	112.73	106.30
1	A	106	TRP	CE2-CD2-CG	-8.00	100.90	107.30
1	A	108	TRP	CE2-CD2-CG	-7.79	101.07	107.30
1	A	51	TRP	CE2-CD2-CG	-7.76	101.09	107.30
1	A	476	GLU	CA-CB-CG	7.58	130.07	113.40
1	A	221	TRP	CD1-CG-CD2	7.39	112.21	106.30
1	A	330	THR	N-CA-C	7.37	130.91	111.00
1	A	516	TRP	CE2-CD2-CG	-7.33	101.44	107.30
1	A	502	TRP	CE2-CD2-CG	-7.26	101.49	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	206	TRP	CE2-CD2-CG	-7.25	101.50	107.30
1	A	256	TRP	CD1-CG-CD2	7.24	112.09	106.30
1	A	449	TRP	CE2-CD2-CG	-7.22	101.52	107.30
1	A	52	TRP	CD1-CG-CD2	7.21	112.07	106.30
1	A	293	TRP	CE2-CD2-CG	-7.18	101.56	107.30
1	A	28	TRP	CG-CD2-CE3	7.10	140.29	133.90
1	A	293	TRP	CD1-CG-CD2	7.06	111.95	106.30
1	A	495	TRP	CE2-CD2-CG	-6.97	101.73	107.30
1	A	52	TRP	CE2-CD2-CG	-6.82	101.84	107.30
1	A	221	TRP	CE2-CD2-CG	-6.72	101.93	107.30
1	A	256	TRP	CE2-CD2-CG	-6.58	102.03	107.30
1	A	106	TRP	CG-CD2-CE3	6.55	139.80	133.90
1	A	467	TRP	CE2-CD2-CG	-6.45	102.14	107.30
1	A	28	TRP	CB-CG-CD1	-6.35	118.74	127.00
1	A	223	THR	N-CA-CB	-6.34	98.26	110.30
1	A	106	TRP	CB-CG-CD1	-6.30	118.81	127.00
1	A	421	MET	CA-CB-CG	6.29	124.00	113.30
1	A	454	TYR	CB-CG-CD2	-6.27	117.24	121.00
1	A	14	TYR	CB-CG-CD2	-6.26	117.25	121.00
1	A	108	TRP	CG-CD2-CE3	6.23	139.51	133.90
1	A	378	TYR	CB-CG-CD2	-6.09	117.35	121.00
1	A	396	LEU	CA-CB-CG	5.97	129.02	115.30
1	A	28	TRP	CG-CD1-NE1	-5.94	104.16	110.10
1	A	108	TRP	CB-CG-CD1	-5.89	119.34	127.00
1	A	397	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	107	VAL	CG1-CB-CG2	-5.75	101.71	110.90
1	A	174	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	467	TRP	CD1-CG-CD2	5.73	110.88	106.30
1	A	165	LEU	CB-CG-CD2	-5.70	101.32	111.00
1	A	454	TYR	N-CA-C	5.62	126.18	111.00
1	A	495	TRP	CG-CD1-NE1	-5.50	104.60	110.10
1	A	37	TRP	CG-CD1-NE1	-5.49	104.61	110.10
1	A	330	THR	N-CA-CB	-5.47	99.91	110.30
1	A	189	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	502	TRP	CG-CD1-NE1	-5.40	104.70	110.10
1	A	94	ASN	CA-C-N	-5.38	105.36	117.20
1	A	206	TRP	CG-CD1-NE1	-5.28	104.82	110.10
1	A	106	TRP	CG-CD1-NE1	-5.28	104.82	110.10
1	A	417	VAL	N-CA-CB	-5.21	100.04	111.50
1	A	44	TYR	CB-CG-CD1	-5.21	117.88	121.00
1	A	310	TYR	CB-CG-CD2	-5.20	117.88	121.00
1	A	493	LYS	CB-CG-CD	-5.17	98.17	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	LEU	N-CA-C	5.14	124.88	111.00
1	A	293	TRP	CB-CG-CD1	-5.13	120.33	127.00
1	A	293	TRP	CG-CD2-CE3	5.09	138.48	133.90
1	A	330	THR	O-C-N	-5.06	114.60	122.70
1	A	206	TRP	CB-CG-CD1	-5.03	120.47	127.00

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	4119	0	3984	52	0
2	A	4	0	3	0	0
3	A	5	0	0	0	0
4	A	1	0	0	0	0
5	A	120	0	0	1	0
All	All	4249	0	3987	52	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (52) 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:365:ASN:HB3	5:A:619:HOH:O	1.85	0.75
1:A:103:ILE:HD11	1:A:108:TRP:CZ2	2.24	0.72
1:A:1:ALA:HA	1:A:387:ASN:HD22	1.56	0.70
1:A:422:GLN:HE22	1:A:510:THR:H	1.40	0.70
1:A:198:PHE:O	1:A:202:LYS:HG2	1.92	0.68
1:A:218:ASN:OD1	1:A:223:THR:HG23	1.99	0.63
1:A:372:ILE:HG23	1:A:377:GLU:HB2	1.83	0.61
1:A:28:TRP:O	1:A:32:GLU:HG3	2.02	0.60
1:A:51:TRP:CZ2	1:A:91:CYS:SG	2.96	0.59
1:A:14:TYR:HD1	1:A:45:ALA:HB3	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:GLN:HE21	1:A:399:GLN:H	1.51	0.59
1:A:156:TYR:O	1:A:159:VAL:HG12	2.03	0.59
1:A:446:LEU:HD21	1:A:473:LEU:HD21	1.86	0.58
1:A:431:THR:HG21	1:A:467:TRP:HE1	1.67	0.58
1:A:295:TYR:HE2	1:A:349:LEU:HD13	1.68	0.57
1:A:172:GLU:HG2	1:A:287:LYS:HD2	1.87	0.55
1:A:90:GLN:HE21	1:A:93:GLY:HA3	1.71	0.55
1:A:27:ASN:ND2	1:A:29:GLU:HB3	2.22	0.55
1:A:27:ASN:HD22	1:A:29:GLU:H	1.56	0.54
1:A:33:ASN:HD22	1:A:36:ARG:HE	1.57	0.54
1:A:269:GLY:O	1:A:273:HIS:HD2	1.90	0.54
1:A:218:ASN:HA	1:A:223:THR:HG22	1.89	0.53
1:A:445:GLU:HG3	1:A:474:PRO:HD3	1.90	0.53
1:A:404:ASN:ND2	1:A:407:LEU:H	2.07	0.52
1:A:336:ASP:HA	1:A:346:PRO:HD2	1.92	0.52
1:A:399:GLN:H	1:A:399:GLN:NE2	2.07	0.51
1:A:442:ASN:ND2	1:A:480:GLU:H	2.08	0.51
1:A:355:THR:O	1:A:359:GLU:HG3	2.11	0.51
1:A:460:TYR:CE2	1:A:462:SER:HA	2.46	0.50
1:A:211:TYR:HB3	1:A:216:GLU:HB3	1.92	0.50
1:A:33:ASN:ND2	1:A:36:ARG:HH21	2.11	0.49
1:A:422:GLN:NE2	1:A:510:THR:H	2.07	0.49
1:A:90:GLN:NE2	1:A:93:GLY:HA3	2.28	0.48
1:A:445:GLU:HG3	1:A:474:PRO:CD	2.44	0.47
1:A:335:THR:HG23	1:A:380:ARG:HD3	1.96	0.47
1:A:385:ALA:HA	1:A:390:PHE:CD1	2.50	0.47
1:A:383:GLU:O	1:A:387:ASN:HB2	2.17	0.45
1:A:107:VAL:O	1:A:110:GLN:HG2	2.17	0.45
1:A:267:LEU:O	1:A:271:LEU:HG	2.17	0.45
1:A:422:GLN:HB2	1:A:473:LEU:HD12	1.99	0.45
1:A:85:ILE:HG12	1:A:164:TYR:HB2	1.99	0.44
1:A:435:ASP:HB3	1:A:485:ILE:CG2	2.46	0.44
1:A:445:GLU:HG3	1:A:474:PRO:HG3	1.99	0.44
1:A:14:TYR:CD1	1:A:45:ALA:HB3	2.50	0.44
1:A:1:ALA:HB3	1:A:5:LYS:O	2.19	0.43
1:A:346:PRO:O	1:A:350:VAL:HG23	2.20	0.42
1:A:404:ASN:HD22	1:A:407:LEU:H	1.68	0.42
1:A:131:ASN:OD1	1:A:133:LEU:HB2	2.20	0.42
1:A:287:LYS:HG2	1:A:288:ILE:N	2.35	0.42
1:A:218:ASN:HA	1:A:223:THR:CG2	2.50	0.41
1:A:22:ILE:HB	1:A:23:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:MET:O	1:A:388:TYR:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	514/516 (100%)	478 (93%)	32 (6%)	4 (1%)	19	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	VAL
1	A	243	ASN
1	A	454	TYR
1	A	92	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	440/440 (100%)	406 (92%)	34 (8%)	13	25

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	15	LEU
1	A	30	THR
1	A	40	GLN
1	A	57	LYS
1	A	112	SER
1	A	130	LEU
1	A	157	LYS
1	A	159	VAL
1	A	165	LEU
1	A	187	PRO
1	A	208	LEU
1	A	224	LYS
1	A	243	ASN
1	A	248	MET
1	A	297	ASN
1	A	316	LEU
1	A	370	LEU
1	A	399	GLN
1	A	404	ASN
1	A	414	LEU
1	A	415	LEU
1	A	417	VAL
1	A	427	LYS
1	A	431	THR
1	A	436	THR
1	A	442	ASN
1	A	470	ASN
1	A	489	ASP
1	A	502	TRP
1	A	504	PRO
1	A	507	LEU
1	A	508	LYS
1	A	510	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	33	ASN
1	A	41	ASN
1	A	90	GLN
1	A	100	ASN

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Mol	Chain	Res	Type
1	A	281	GLN
1	A	292	HIS
1	A	297	ASN
1	A	387	ASN
1	A	399	GLN
1	A	404	ASN
1	A	405	ASN
1	A	422	GLN
1	A	442	ASN
1	A	463	HIS
1	A	470	ASN
1	A	496	GLN
1	A	512	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 is 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	$\#|Z| > 2$
2	ACT	A	920	-	3,3,3	1.02	0	3,3,3	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z \rvert > 2$	Counts	RMSZ	$\#\lvert Z \rvert > 2$
3	SO4	A	921	-	4,4,4	0.27	0	6,6,6	0.18	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.