



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:34 PM GMT

PDB ID : 1BG9  
Title : BARLEY ALPHA-AMYLASE WITH SUBSTRATE ANALOGUE ACAR-BOSE  
Authors : Kadziola, A.; Haser, R.  
Deposited on : 1998-06-05  
Resolution : 2.80 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](mailto: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.

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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

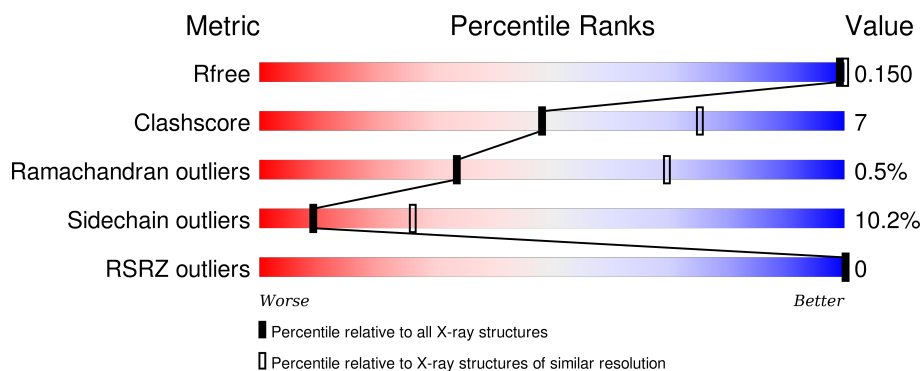
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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  $\geq 3$ , 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	403	

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	DAF	A	800	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BGC	A	801	-	-	-	X
4	AF1	A	803	X	-	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3390 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 1,4-ALPHA-D-GLUCAN GLUCANOHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	0	0	0
			3184	2040	552	583	9			

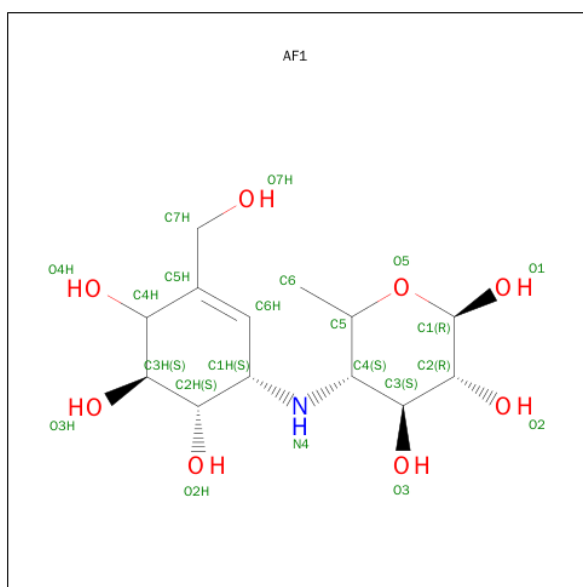
- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			33	19	1	13		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Ca	0	0
			3	3		

- Molecule 4 is 4-DEOXY-4-((5-HYDROXYMETHYL-2,3,4-TRIHYDROXYCYCLOHEX-5,6-ENYL)AMINO)FRUCTOSE (three-letter code: AF1) (formula: C<sub>13</sub>H<sub>23</sub>NO<sub>8</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			22	13	1	8		

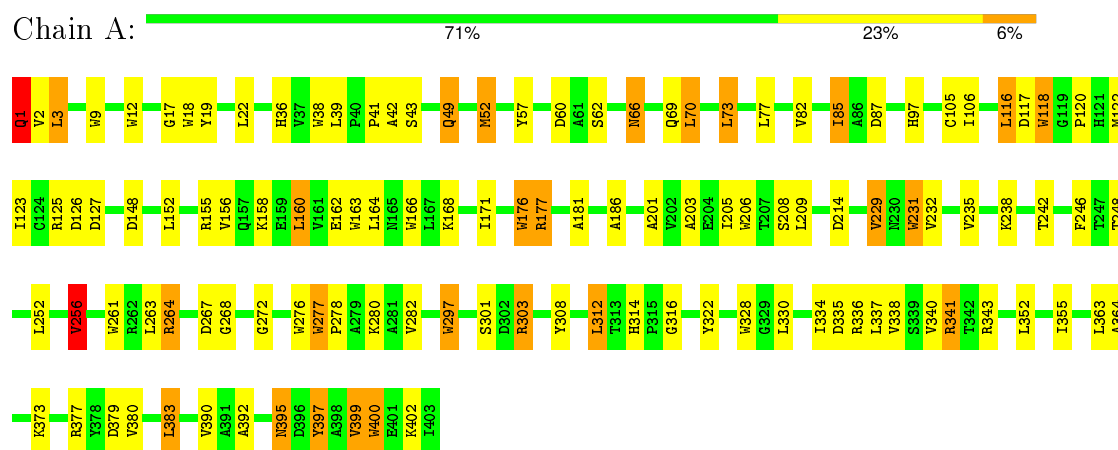
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	148	Total	O	0	0
			148	148		

### 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: 1,4-ALPHA-D-GLUCAN GLUCANOHYDROLASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.20 Å   135.20 Å   79.60 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	10.00 – 2.80 9.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	86.4 (10.00-2.80) 86.4 (9.98-2.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.99 (at 2.79 Å)	Xtriage
Refinement program	X-PLOR 2.1	Depositor
R, $R_{free}$	0.151 , 0.249 0.151 , 0.150	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	28.9	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 55.0	EDS
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 17688 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3390	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CA, BGC, DAF, AF1

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	1.01	1/3281 (0.0%)	1.68	74/4459 (1.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	328	TRP	CG-CD2	-5.14	1.34	1.43

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	ARG	NE-CZ-NH2	-11.61	114.49	120.30
1	A	341	ARG	NE-CZ-NH2	-10.43	115.08	120.30
1	A	303	ARG	NE-CZ-NH2	-10.10	115.25	120.30
1	A	12	TRP	CD1-CG-CD2	9.32	113.75	106.30
1	A	341	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	A	328	TRP	CD1-CG-CD2	8.74	113.29	106.30
1	A	166	TRP	CD1-CG-CD2	8.66	113.23	106.30
1	A	38	TRP	CD1-CG-CD2	8.65	113.22	106.30
1	A	176	TRP	CD1-CG-CD2	8.63	113.20	106.30
1	A	277	TRP	CD1-CG-CD2	8.61	113.19	106.30
1	A	177	ARG	NE-CZ-NH1	8.43	124.51	120.30
1	A	9	TRP	CD1-CG-CD2	8.42	113.03	106.30
1	A	52	MET	CG-SD-CE	-8.01	87.39	100.20
1	A	297	TRP	CD1-CG-CD2	7.92	112.64	106.30
1	A	400	TRP	CD1-CG-CD2	7.86	112.59	106.30
1	A	261	TRP	CD1-CG-CD2	7.86	112.59	106.30
1	A	176	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	A	163	TRP	CD1-CG-CD2	7.57	112.36	106.30
1	A	18	TRP	CD1-CG-CD2	7.46	112.27	106.30
1	A	297	TRP	CE2-CD2-CG	-7.38	101.40	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	TRP	CE2-CD2-CG	-7.36	101.42	107.30
1	A	12	TRP	CE2-CD2-CG	-7.34	101.42	107.30
1	A	400	TRP	CE2-CD2-CG	-7.34	101.42	107.30
1	A	118	TRP	CE2-CD2-CG	-7.21	101.53	107.30
1	A	231	TRP	CD1-CG-CD2	7.13	112.00	106.30
1	A	261	TRP	CE2-CD2-CG	-7.10	101.62	107.30
1	A	118	TRP	CD1-CG-CD2	7.09	111.97	106.30
1	A	328	TRP	CE2-CD2-CG	-6.96	101.73	107.30
1	A	397	TYR	CB-CG-CD2	-6.92	116.84	121.00
1	A	166	TRP	CE2-CD2-CG	-6.91	101.77	107.30
1	A	277	TRP	CE2-CD2-CG	-6.84	101.83	107.30
1	A	38	TRP	CE2-CD2-CG	-6.81	101.85	107.30
1	A	402	LYS	O-C-N	6.74	133.48	122.70
1	A	163	TRP	CE2-CD2-CG	-6.73	101.92	107.30
1	A	377	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	A	322	TYR	CB-CG-CD1	-6.70	116.98	121.00
1	A	18	TRP	CE2-CD2-CG	-6.67	101.96	107.30
1	A	12	TRP	CG-CD1-NE1	-6.29	103.81	110.10
1	A	231	TRP	CE2-CD2-CG	-6.28	102.28	107.30
1	A	276	TRP	CD1-CG-CD2	6.24	111.29	106.30
1	A	206	TRP	CE2-CD2-CG	-6.16	102.37	107.30
1	A	19	TYR	CB-CG-CD2	-6.13	117.32	121.00
1	A	176	TRP	CG-CD1-NE1	-6.11	103.99	110.10
1	A	297	TRP	CG-CD2-CE3	6.10	139.39	133.90
1	A	206	TRP	CD1-CG-CD2	6.08	111.16	106.30
1	A	277	TRP	CG-CD1-NE1	-6.05	104.05	110.10
1	A	60	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	A	1	GLN	N-CA-C	-5.97	94.89	111.00
1	A	276	TRP	CE2-CD2-CG	-5.88	102.60	107.30
1	A	38	TRP	CG-CD1-NE1	-5.87	104.23	110.10
1	A	127	ASP	CB-CG-OD1	5.83	123.54	118.30
1	A	60	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	261	TRP	CB-CG-CD1	-5.73	119.55	127.00
1	A	162	GLU	CA-CB-CG	5.63	125.79	113.40
1	A	166	TRP	CG-CD1-NE1	-5.57	104.53	110.10
1	A	328	TRP	CG-CD1-NE1	-5.54	104.56	110.10
1	A	343	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	256	VAL	N-CA-CB	-5.52	99.36	111.50
1	A	264	ARG	N-CA-C	-5.46	96.27	111.00
1	A	18	TRP	CG-CD1-NE1	-5.38	104.72	110.10
1	A	395	ASN	N-CA-C	5.34	125.41	111.00
1	A	3	LEU	CB-CG-CD1	-5.31	101.98	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	ASP	CA-CB-CG	5.26	124.98	113.40
1	A	231	TRP	CG-CD1-NE1	-5.26	104.84	110.10
1	A	155	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	9	TRP	CG-CD1-NE1	-5.25	104.85	110.10
1	A	118	TRP	CG-CD2-CE3	5.19	138.57	133.90
1	A	297	TRP	CG-CD1-NE1	-5.18	104.92	110.10
1	A	85	ILE	CB-CG1-CD1	-5.15	99.48	113.90
1	A	256	VAL	CA-CB-CG2	-5.06	103.31	110.90
1	A	3	LEU	CA-CB-CG	5.03	126.87	115.30
1	A	117	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	261	TRP	CG-CD1-NE1	-5.03	105.07	110.10
1	A	163	TRP	CG-CD1-NE1	-5.02	105.08	110.10

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	3184	0	3044	45	0
2	A	33	0	25	1	0
3	A	3	0	0	0	0
4	A	22	0	21	0	0
5	A	148	0	0	2	0
All	All	3390	0	3090	46	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 7.

All (46) 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:105:CYS:SG	1:A:120:PRO:HG3	2.36	0.66
1:A:229:VAL:HG22	1:A:277:TRP:HE3	1.60	0.65
1:A:77:LEU:HB3	1:A:82:VAL:HG22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:GLN:NE2	1:A:49:GLN:H	2.01	0.59
1:A:390:VAL:HA	1:A:400:TRP:HA	1.86	0.56
1:A:186:ALA:HB1	1:A:235:VAL:HG23	1.88	0.55
1:A:256:VAL:HG13	1:A:303:ARG:CD	2.37	0.54
1:A:355:ILE:HG21	1:A:363:LEU:HD23	1.89	0.54
1:A:41:PRO:HG3	1:A:87:ASP:HB3	1.90	0.54
1:A:118:TRP:HB3	1:A:122:MET:SD	2.49	0.53
1:A:256:VAL:HG13	1:A:303:ARG:HD2	1.92	0.52
1:A:308:TYR:O	1:A:312:LEU:HB2	2.09	0.52
1:A:3:LEU:HD22	1:A:36:HIS:HB2	1.92	0.52
1:A:1:GLN:OE1	1:A:1:GLN:N	2.45	0.50
1:A:66:ASN:ND2	1:A:69:GLN:H	2.11	0.48
1:A:97:HIS:HB2	1:A:106:ILE:HB	1.94	0.48
1:A:373:LYS:O	1:A:397:TYR:HA	2.13	0.48
1:A:392:ALA:HB3	1:A:399:VAL:HG13	1.94	0.48
1:A:158:LYS:HA	1:A:158:LYS:HE2	1.95	0.48
2:A:800:DAF:H6	2:A:800:DAF:H3H	1.97	0.47
1:A:264:ARG:HG2	1:A:268:GLY:HA2	1.96	0.47
1:A:380:VAL:O	1:A:383:LEU:HD12	2.14	0.47
1:A:232:VAL:HG11	1:A:280:LYS:HG3	1.96	0.47
1:A:203:ALA:HB2	1:A:231:TRP:CH2	2.50	0.46
1:A:57:TYR:CE2	1:A:116:LEU:HD22	2.50	0.46
1:A:242:THR:HG22	1:A:280:LYS:HA	1.99	0.45
1:A:248:THR:O	1:A:252:LEU:HB2	2.18	0.44
1:A:246:PHE:HD2	1:A:297:TRP:HZ3	1.66	0.44
1:A:248:THR:OG1	1:A:272:GLY:HA3	2.18	0.43
1:A:70:LEU:HD13	1:A:171:ILE:HG21	2.00	0.43
1:A:156:VAL:O	1:A:160:LEU:HB2	2.18	0.43
1:A:314:HIS:O	1:A:341:ARG:NH2	2.52	0.42
1:A:252:LEU:O	1:A:256:VAL:HB	2.20	0.42
1:A:352:LEU:HD11	1:A:364:ALA:HB1	2.02	0.42
1:A:278:PRO:O	1:A:316:GLY:HA2	2.20	0.42
1:A:17:GLY:HA2	5:A:621:HOH:O	2.20	0.42
1:A:176:TRP:O	1:A:201:ALA:HA	2.20	0.41
1:A:42:ALA:O	1:A:62:SER:HB2	2.20	0.41
1:A:22:LEU:HA	1:A:22:LEU:HD12	1.86	0.41
1:A:126:ASP:HB2	5:A:610:HOH:O	2.20	0.41
1:A:160:LEU:HA	1:A:160:LEU:HD12	1.86	0.41
1:A:336:ARG:O	1:A:340:VAL:HG23	2.21	0.41
1:A:181:ALA:HB3	1:A:205:ILE:HD13	2.02	0.40
1:A:22:LEU:HD23	1:A:73:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:PRO:HA	1:A:123:ILE:HD12	2.04	0.40
1:A:334:ILE:O	1:A:338:VAL:HG23	2.21	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	401/403 (100%)	381 (95%)	18 (4%)	2 (0%)	34 69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	ASP
1	A	125	ARG

### 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	322/322 (100%)	289 (90%)	33 (10%)	9 26

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	2	VAL
1	A	39	LEU
1	A	43	SER
1	A	49	GLN
1	A	52	MET
1	A	66	ASN
1	A	70	LEU
1	A	73	LEU
1	A	85	ILE
1	A	116	LEU
1	A	148	ASP
1	A	152	LEU
1	A	160	LEU
1	A	164	LEU
1	A	168	LYS
1	A	177	ARG
1	A	208	SER
1	A	209	LEU
1	A	229	VAL
1	A	238	LYS
1	A	256	VAL
1	A	263	LEU
1	A	282	VAL
1	A	301	SER
1	A	312	LEU
1	A	330	LEU
1	A	335	ASP
1	A	337	LEU
1	A	379	ASP
1	A	383	LEU
1	A	395	ASN
1	A	399	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	66	ASN
1	A	97	HIS
1	A	226	GLN
1	A	230	ASN
1	A	306	GLN

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Mol	Chain	Res	Type
1	A	382	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 ⓘ

2 carbohydrates 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	DAF	A	800	2	18,22,23	5.18	7 (38%)	14,32,34	2.12	5 (35%)
2	BGC	A	801	2	12,12,12	0.64	0	17,17,17	2.21	7 (41%)

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	DAF	A	800	2	-	1/5/43/46	0/2/2/2
2	BGC	A	801	2	-	0/2/22/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	DAF	C1H-C6H	-2.15	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	DAF	C3H-C4H	3.11	1.57	1.52
2	A	800	DAF	C7H-C5H	3.28	1.55	1.45
2	A	800	DAF	C5H-C4H	4.18	1.54	1.44
2	A	800	DAF	O7H-C7H	9.06	1.43	1.22
2	A	800	DAF	O4H-C4H	11.52	1.43	1.22
2	A	800	DAF	C6-C5	14.86	1.52	1.31

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	DAF	O7H-C7H-C5H	-4.01	116.22	125.38
2	A	800	DAF	C1H-C2H-C3H	-3.66	103.53	110.20
2	A	801	BGC	C4-C3-C2	-2.47	106.18	110.79
2	A	801	BGC	O4-C4-C3	-2.37	105.00	110.34
2	A	801	BGC	O2-C2-C1	2.26	114.79	109.82
2	A	801	BGC	C1-O5-C5	2.27	117.66	113.47
2	A	800	DAF	O2H-C2H-C3H	2.39	113.79	109.49
2	A	800	DAF	O5-C1-C2	3.06	114.64	111.06
2	A	800	DAF	O2H-C2H-C1H	3.21	115.71	109.16
2	A	801	BGC	O5-C5-C6	3.36	114.84	106.36
2	A	801	BGC	C6-C5-C4	3.59	121.88	113.02
2	A	801	BGC	O5-C5-C4	5.22	119.48	109.68

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	800	DAF	C6H-C1H-N4-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	DAF	1	0

## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	AF1	A	803	-	22,23,23	1.83	6 (27%)	22,34,34	2.53	8 (36%)

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	AF1	A	803	-	2/2/10/12	0/6/46/46	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	AF1	C1H-C6H	-4.57	1.43	1.50
4	A	803	AF1	C1H-N4	-2.56	1.42	1.47
4	A	803	AF1	C4H-C5H	2.02	1.57	1.50
4	A	803	AF1	C7H-C5H	2.08	1.55	1.50
4	A	803	AF1	C3H-C4H	2.54	1.56	1.53
4	A	803	AF1	C6H-C5H	4.32	1.39	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	AF1	C3-C4-N4	-5.09	96.31	111.38
4	A	803	AF1	C2H-C3H-C4H	-2.20	108.05	110.73
4	A	803	AF1	O3H-C3H-C4H	2.07	113.23	109.49
4	A	803	AF1	O1-C1-O5	2.42	116.86	110.25
4	A	803	AF1	O3-C3-C2	3.17	117.48	110.34
4	A	803	AF1	O5-C5-C6	4.07	115.53	106.64
4	A	803	AF1	O4H-C4H-C3H	4.46	119.03	109.95
4	A	803	AF1	O4H-C4H-C5H	6.71	124.81	110.36

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	803	AF1	C5

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Mol	Chain	Res	Type	Atom
4	A	803	AF1	C4H

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	403/403 (100%)	-1.41	0 100 100	4, 14, 46, 80	0

There are no RSRZ outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
2	BGC	A	801	12/12	0.98	0.13	3.62	33,37,40,44	0
2	DAF	A	800	21/22	0.97	0.10	3.20	24,33,36,36	0

### 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	AF1	A	803	22/22	0.94	0.13	1.46	35,44,54,61	0
3	CA	A	501	1/1	0.98	0.07	-0.20	15,15,15,15	0
3	CA	A	500	1/1	1.00	0.05	-1.41	5,5,5,5	0
3	CA	A	502	1/1	0.95	0.05	-1.42	17,17,17,17	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.