



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:16 AM GMT

PDB ID : 3OLG
Title : Structures of human pancreatic alpha-amylase in complex with acarviosatin III03
Authors : Qin, X.; Ren, L.
Deposited on : 2010-08-26
Resolution : 2.30 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 ⓘ symbol.

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

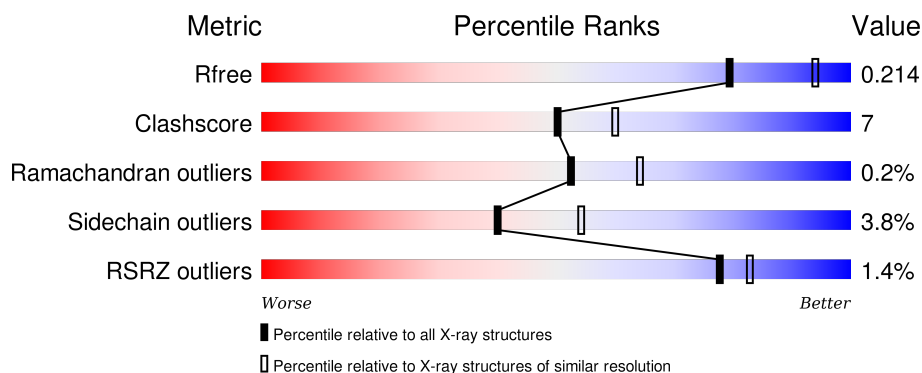
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 $\leq 5\%$. 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	496	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; text-align: center;">%</div> <div style="position: absolute; top: 10px; left: 0; width: 100%; text-align: center;">85% 13% •</div> </div> </div>

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
10	GLC	A	512	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	GLC	A	514	X	-	-	-
11	BGC	A	515	-	-	-	X
6	HSD	A	503	-	-	-	X
7	G6D	A	504	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 4384 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 Pancreatic alpha-amylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	0	0
			3939	2492	695	731	21			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	287	MET	VAL	ENGINEERED MUTATION	UNP P04746

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

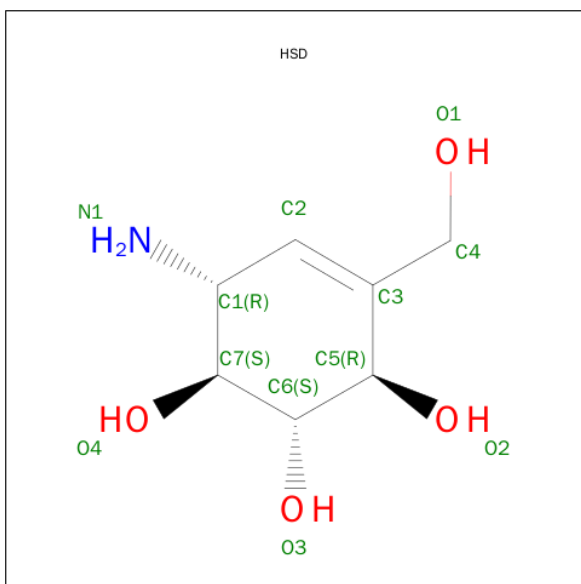
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is SUGAR (6-AMINO-4-HYDROXYMETHYL-CYCLOHEX-4-ENE-1,2,3-TRIOL) (three-letter code: HSD) (formula: $C_7H_{13}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			12	7	1	4		

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	3	Total	C	N	O	0	0
			32	19	1	12		

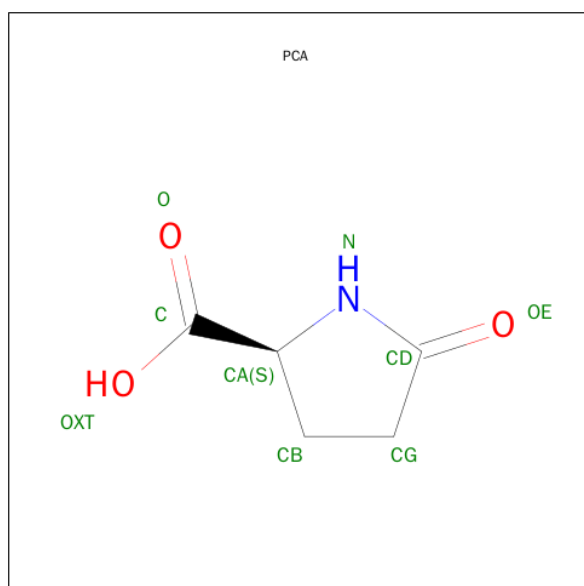
- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	3	Total	C	O	0	0
			32	18	14		

- Molecule 8 is a polymer of unknown type called SUGAR (4-MER).

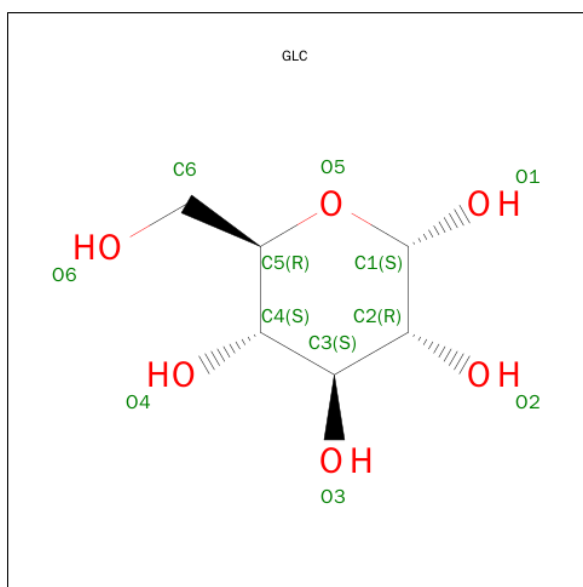
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	4	Total	C	O	0	0
			45	24	21		

- Molecule 9 is PYROGLUTAMIC ACID (three-letter code: PCA) (formula: $C_5H_7NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			8	5	1	2		

- Molecule 10 is SUGAR (ALPHA-D-GLUCOSE) (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 11 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	3	Total	C	O	0	0
			34	18	16		

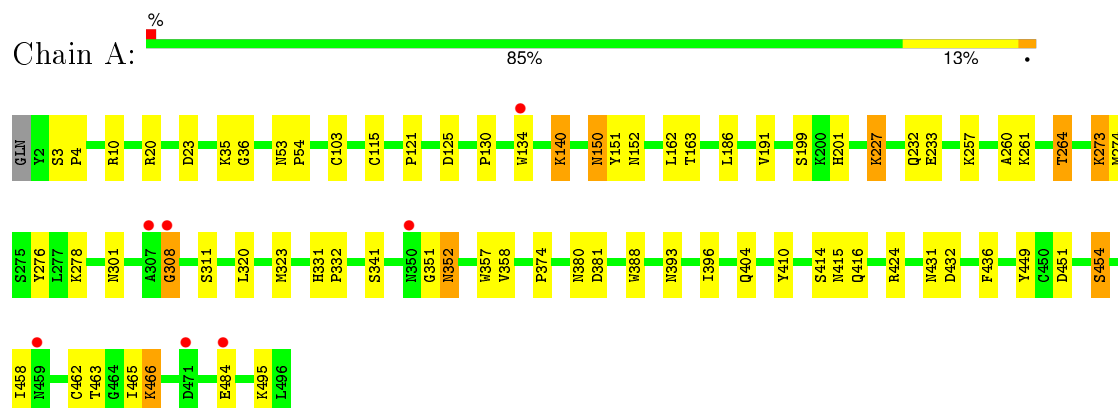
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	263	Total	O	0	0
			263	263		

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: Pancreatic alpha-amylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.38 Å 74.53 Å 135.74 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.87 – 2.30 40.87 – 2.29	Depositor EDS
% Data completeness (in resolution range)	94.6 (40.87-2.30) 94.0 (40.87-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.93 (at 2.29 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.193 , 0.216 0.190 , 0.214	Depositor DCC
R_{free} test set	1176 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 24551 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4384	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, HSD, CL, CA, GLC, G6D, SO4, PCA

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	0.40	0/4053	0.66	0/5503

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	A	1	0

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	A	514	GLC	C1

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	3939	0	3711	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	5	0	0	0	0
5	A	12	0	11	2	0
6	A	32	0	27	1	0
7	A	32	0	28	0	0
8	A	45	0	39	1	0
9	A	8	0	5	0	0
10	A	12	0	12	1	0
11	A	34	0	30	1	0
12	A	263	0	0	7	0
All	All	4384	0	3863	56	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 (56) 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:163:THR:HB	5:A:500:HSD:H2	1.40	0.87
1:A:150:ASN:ND2	1:A:152:ASN:H	1.95	0.65
1:A:257:LYS:O	1:A:261:LYS:HG2	1.97	0.65
1:A:264:THR:HG22	1:A:311:SER:CB	2.28	0.63
1:A:260:ALA:O	1:A:264:THR:HG23	2.04	0.58
1:A:416:GLN:HG3	1:A:432:ASP:OD2	2.04	0.57
1:A:484:GLU:HB3	12:A:1059:HOH:O	2.04	0.57
1:A:273:LYS:HA	1:A:415:ASN:HD21	1.71	0.56
1:A:451:ASP:OD2	1:A:454:SER:HB2	2.06	0.56
1:A:393:ASN:O	1:A:396:ILE:HG23	2.05	0.56
1:A:20:ARG:NH1	1:A:23:ASP:OD2	2.40	0.55
1:A:352:ASN:N	1:A:352:ASN:OD1	2.40	0.54
1:A:462:CYS:HB2	1:A:466:LYS:HD2	1.89	0.54
1:A:415:ASN:HB3	1:A:431:ASN:HB3	1.91	0.53
1:A:320:LEU:HA	1:A:323:MET:HE3	1.91	0.53
1:A:233:GLU:OE2	6:A:503:HSD:N1	2.43	0.52
1:A:103:CYS:SG	1:A:121:PRO:HG3	2.50	0.51
1:A:162:LEU:HD22	1:A:201:HIS:CD2	2.45	0.51
1:A:404:GLN:HG3	1:A:424:ARG:HG3	1.93	0.51
1:A:227:LYS:HB2	12:A:965:HOH:O	2.10	0.50
11:A:515:BGC:H1	12:A:990:HOH:O	2.10	0.50
1:A:274:MET:HG3	12:A:572:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LYS:NZ	12:A:991:HOH:O	2.43	0.50
1:A:393:ASN:O	1:A:396:ILE:CG2	2.60	0.49
1:A:301:ASN:HB2	1:A:308:GLY:HA3	1.94	0.49
1:A:393:ASN:HA	1:A:396:ILE:HG22	1.95	0.49
1:A:273:LYS:HB2	1:A:414:SER:O	2.13	0.48
8:A:509:GLC:O5	8:A:510:BGC:H6C2	2.14	0.48
1:A:274:MET:H	1:A:415:ASN:HD22	1.62	0.47
1:A:374:PRO:HG2	12:A:1066:HOH:O	2.14	0.47
1:A:351:GLY:C	1:A:352:ASN:OD1	2.54	0.46
1:A:396:ILE:HG23	12:A:715:HOH:O	2.15	0.46
1:A:264:THR:HG22	1:A:311:SER:OG	2.15	0.46
1:A:199:SER:CB	1:A:232:GLN:HB3	2.46	0.46
1:A:462:CYS:SG	1:A:466:LYS:HD2	2.55	0.45
1:A:163:THR:HB	5:A:500:HSD:N1	2.21	0.45
1:A:150:ASN:HD21	1:A:152:ASN:HB2	1.82	0.45
1:A:3:SER:HA	1:A:4:PRO:HD3	1.82	0.44
1:A:186:LEU:O	1:A:191:VAL:HG13	2.17	0.44
1:A:53:ASN:HA	1:A:54:PRO:C	2.35	0.44
1:A:150:ASN:HD22	1:A:151:TYR:N	2.16	0.43
1:A:274:MET:H	1:A:415:ASN:ND2	2.17	0.42
1:A:357:TRP:CE3	1:A:358:VAL:HA	2.53	0.42
1:A:150:ASN:HD22	1:A:150:ASN:C	2.22	0.42
1:A:10:ARG:NH1	1:A:36:GLY:HA2	2.34	0.41
1:A:380:ASN:O	1:A:381:ASP:HB2	2.19	0.41
1:A:410:TYR:C	1:A:410:TYR:CD1	2.93	0.41
1:A:273:LYS:HD3	1:A:276:TYR:CZ	2.55	0.41
1:A:449:TYR:CE2	1:A:495:LYS:HB2	2.56	0.41
1:A:261:LYS:HD2	1:A:261:LYS:HA	1.78	0.41
1:A:273:LYS:HA	1:A:415:ASN:ND2	2.36	0.41
1:A:331:HIS:CG	1:A:332:PRO:HD2	2.56	0.41
1:A:465:ILE:CG2	1:A:466:LYS:N	2.83	0.41
1:A:388:TRP:CD1	10:A:512:GLC:H61	2.56	0.40
1:A:458:ILE:HD12	1:A:463:THR:HG21	2.03	0.40
1:A:462:CYS:CB	1:A:466:LYS:HD2	2.52	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	493/496 (99%)	471 (96%)	21 (4%)	1 (0%)	52	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	308	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	418/419 (100%)	402 (96%)	16 (4%)	40	54

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LYS
1	A	115	CYS
1	A	125	ASP
1	A	130	PRO
1	A	134	TRP
1	A	140	LYS
1	A	150	ASN
1	A	227	LYS
1	A	264	THR
1	A	273	LYS

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Mol	Chain	Res	Type
1	A	278	LYS
1	A	341	SER
1	A	352	ASN
1	A	436	PHE
1	A	454	SER
1	A	466	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	15	HIS
1	A	53	ASN
1	A	150	ASN
1	A	152	ASN
1	A	216	ASN
1	A	415	ASN
1	A	476	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 ⓘ

13 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
6	G6D	A	501	5,6	9,9,11	0.62	0	10,12,16	1.89	3 (30%)
6	GLC	A	502	6	11,11,12	0.53	0	14,15,17	1.08	2 (14%)
6	HSD	A	503	7,6	11,12,12	1.53	1 (9%)	9,17,17	3.07	3 (33%)
7	G6D	A	504	7,6	9,9,11	0.54	0	10,12,16	0.97	0
7	GLC	A	505	7	11,11,12	0.57	0	14,15,17	0.93	1 (7%)
7	BGC	A	506	7	12,12,12	0.62	0	17,17,17	1.19	2 (11%)
8	GLC	A	507	8	11,11,12	0.42	0	14,15,17	0.36	0
8	GLC	A	508	8	11,11,12	0.30	0	14,15,17	0.50	0
8	GLC	A	509	8	11,11,12	0.42	0	14,15,17	0.81	1 (7%)
8	BGC	A	510	8	12,12,12	1.21	2 (16%)	17,17,17	2.17	4 (23%)
11	GLC	A	513	11	11,11,12	0.72	0	14,15,17	1.78	2 (14%)
11	GLC	A	514	11	11,11,12	1.19	2 (18%)	14,15,17	1.71	3 (21%)
11	BGC	A	515	11	12,12,12	1.48	3 (25%)	17,17,17	2.99	9 (52%)

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
6	G6D	A	501	5,6	-	0/0/13/20	0/1/1/1
6	GLC	A	502	6	-	0/2/19/22	0/1/1/1
6	HSD	A	503	7,6	-	0/2/22/22	0/1/1/1
7	G6D	A	504	7,6	-	0/0/13/20	0/1/1/1
7	GLC	A	505	7	-	0/2/19/22	0/1/1/1
7	BGC	A	506	7	-	0/2/22/22	0/1/1/1
8	GLC	A	507	8	-	0/2/19/22	0/1/1/1
8	GLC	A	508	8	-	0/2/19/22	0/1/1/1
8	GLC	A	509	8	-	0/2/19/22	0/1/1/1
8	BGC	A	510	8	-	0/2/22/22	0/1/1/1
11	GLC	A	513	11	-	0/2/19/22	0/1/1/1
11	GLC	A	514	11	1/1/4/5	0/2/19/22	0/1/1/1
11	BGC	A	515	11	-	0/2/22/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	514	GLC	C4-C5	-2.13	1.48	1.53
11	A	514	GLC	C1-C2	2.01	1.57	1.52
8	A	510	BGC	C4-C3	2.11	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	515	BGC	C1-C2	2.22	1.57	1.52
8	A	510	BGC	O5-C1	2.40	1.47	1.43
11	A	515	BGC	O5-C1	2.94	1.48	1.43
11	A	515	BGC	O5-C5	2.98	1.51	1.44
6	A	503	HSD	C2-C3	4.42	1.39	1.32

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	515	BGC	C4-C3-C2	-8.86	94.26	110.79
8	A	510	BGC	C1-C2-C3	-6.29	101.07	110.43
6	A	501	G6D	C6A-C5A-C4A	-3.67	107.26	113.38
11	A	514	GLC	C2-C3-C4	-3.29	105.46	111.04
7	A	506	BGC	C1-C2-C3	-3.13	105.77	110.43
6	A	501	G6D	O5-C1-C2	-3.05	105.91	110.86
11	A	515	BGC	C3-C4-C5	-2.98	105.00	110.20
8	A	510	BGC	C1-O5-C5	-2.89	108.12	113.47
6	A	501	G6D	O3A-C3A-C2	-2.75	104.11	110.27
8	A	509	GLC	C2-C3-C4	-2.35	107.06	111.04
6	A	503	HSD	O4-C7-C1	2.05	113.02	108.99
11	A	515	BGC	O3-C3-C4	2.05	114.95	110.34
6	A	502	GLC	O5-C1-C2	2.06	114.21	110.86
8	A	510	BGC	C3-C4-C5	2.14	113.93	110.20
11	A	515	BGC	O5-C5-C4	2.17	113.75	109.68
11	A	515	BGC	C1-O5-C5	2.28	117.69	113.47
6	A	502	GLC	C1-C2-C3	2.31	112.27	109.54
7	A	506	BGC	C3-C4-C5	2.55	114.64	110.20
11	A	515	BGC	O5-C1-C2	2.61	113.95	109.80
11	A	514	GLC	C1-O5-C5	2.81	115.81	112.25
7	A	505	GLC	C1-C2-C3	2.85	112.92	109.54
11	A	514	GLC	O5-C1-C2	2.93	115.61	110.86
11	A	515	BGC	C6-C5-C4	3.23	120.98	113.02
8	A	510	BGC	C6-C5-C4	3.25	121.04	113.02
11	A	513	GLC	C1-O5-C5	3.34	116.48	112.25
11	A	515	BGC	O4-C4-C3	3.38	117.94	110.34
11	A	515	BGC	C1-C2-C3	4.06	116.46	110.43
6	A	503	HSD	O4-C7-C6	4.27	119.95	110.34
11	A	513	GLC	O5-C1-C2	4.84	118.71	110.86
6	A	503	HSD	C7-C1-N1	7.45	126.55	111.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	A	514	GLC	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	503	HSD	1	0
8	A	509	GLC	1	0
8	A	510	BGC	1	0
11	A	515	BGC	1	0

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	SO4	A	499	-	4,4,4	0.22	0	6,6,6	0.09	0
5	HSD	A	500	6	11,12,12	1.55	1 (9%)	9,17,17	4.03	7 (77%)
9	PCA	A	511	1	7,8,9	0.68	0	9,10,12	1.81	3 (33%)
10	GLC	A	512	-	12,12,12	0.52	0	17,17,17	0.50	0

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	SO4	A	499	-	-	0/0/0/0	0/0/0/0
5	HSD	A	500	6	-	0/2/22/22	0/1/1/1
9	PCA	A	511	1	-	0/0/11/13	0/1/1/1
10	GLC	A	512	-	-	0/2/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	500	HSD	C2-C3	4.68	1.39	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	511	PCA	O-C-CA	-3.34	116.62	125.44
5	A	500	HSD	O2-C5-C3	-2.90	104.12	110.36
5	A	500	HSD	C7-C6-C5	-2.84	107.26	110.73
9	A	511	PCA	CB-CA-C	-2.55	109.27	112.76
9	A	511	PCA	CB-CG-CD	-2.47	99.21	104.22
5	A	500	HSD	O1-C4-C3	2.03	117.02	112.12
5	A	500	HSD	O2-C5-C6	2.63	115.30	109.95
5	A	500	HSD	O3-C6-C5	3.39	115.61	109.49
5	A	500	HSD	O4-C7-C6	6.14	124.16	110.34
5	A	500	HSD	C7-C1-N1	8.08	127.82	111.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	500	HSD	2	0
10	A	512	GLC	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	495/496 (99%)	-0.31	7 (1%) 78 83	13, 22, 33, 45	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	484	GLU	5.1
1	A	308	GLY	4.1
1	A	459	ASN	3.6
1	A	307	ALA	3.1
1	A	471	ASP	2.7
1	A	350	ASN	2.7
1	A	134	TRP	2.3

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](#)

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, 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	LLDF	B-factors(Å ²)	Q<0.9
6	HSD	A	503	12/12	0.81	0.21	6.72	22,23,25,27	0
11	BGC	A	515	12/12	0.77	0.29	3.92	32,37,38,42	0
7	G6D	A	504	9/11	0.92	0.14	2.32	22,24,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	G6D	A	501	9/11	0.93	0.13	1.99	28,29,31,33	0
6	GLC	A	502	11/12	0.96	0.11	1.89	19,22,24,26	0
7	BGC	A	506	12/12	0.71	0.22	1.03	36,42,43,43	0
8	GLC	A	508	11/12	0.91	0.18	0.68	36,40,42,45	0
7	GLC	A	505	11/12	0.94	0.15	0.26	28,32,33,34	0
8	BGC	A	510	12/12	0.63	0.53	-	20,20,20,20	0
11	GLC	A	514	11/12	0.66	0.31	-	42,44,46,48	0
11	GLC	A	513	11/12	0.44	0.68	-	20,20,20,20	0
8	GLC	A	509	11/12	0.81	0.18	-	40,41,42,42	0
8	GLC	A	507	11/12	0.80	0.29	-	44,46,48,51	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, 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	LLDF	B-factors(\AA^2)	Q<0.9
10	GLC	A	512	12/12	0.80	0.41	15.28	14,17,21,23	0
9	PCA	A	511	8/9	0.95	0.14	0.23	24,25,25,25	0
3	CL	A	498	1/1	1.00	0.13	-0.08	17,17,17,17	0
2	CA	A	497	1/1	0.98	0.09	-0.78	29,29,29,29	0
5	HSD	A	500	12/12	0.67	0.36	-	39,47,48,48	0
4	SO4	A	499	5/5	0.78	0.32	-	78,78,79,80	0

6.5 Other polymers ⓘ

There are no such residues in this entry.