



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:45 AM GMT

PDB ID : 3FU8
Title : Melanocarpus albomyces laccase crystal soaked (10 sec) with 2,6-dimethoxyphenol
Authors : Kallio, J.P.; Hakulinen, N.; Rouvinen, J.
Deposited on : 2009-01-14
Resolution : 1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

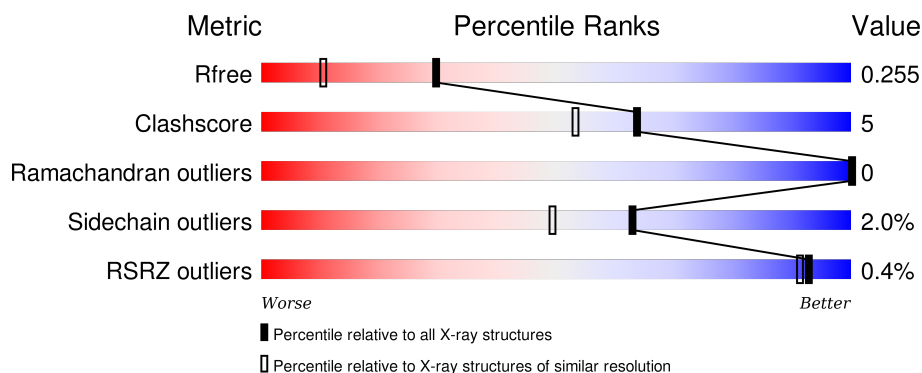
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 ≥ 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	559	 89% 11%
1	B	559	 88% 12%

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	GOL	A	3902[A]	-	-	-	X
4	NAG	A	700	-	-	-	X
4	NAG	A	750	-	-	-	X
4	NAG	B	2760	-	-	-	X
4	NAG	B	700	-	-	-	X
5	MAN	A	712	X	-	-	-
5	MAN	B	712	X	-	-	-
6	NAG	A	720	-	-	-	X
6	NAG	A	760	-	-	-	X
7	MAN	A	732	X	-	-	-
7	MAN	B	732	X	-	-	-
9	3DM	A	2900	-	-	-	X
9	3DM	B	2910	-	-	-	X

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 10570 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 Laccase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	559	Total	C	N	O	S	0	4	0
			4394	2776	763	839	16			
1	B	559	Total	C	N	O	S	0	3	0
			4393	2776	765	836	16			

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	4	Total	Cu	0	0
			4	4		
2	A	4	Total	Cu	0	0
			4	4		

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

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

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	4	Total	C	N	O	0	0
			50	28	2	20		
5	B	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	2	Total	C	N	O	0	0
			28	16	2	10		
6	A	2	Total	C	N	O	0	0
			28	16	2	10		

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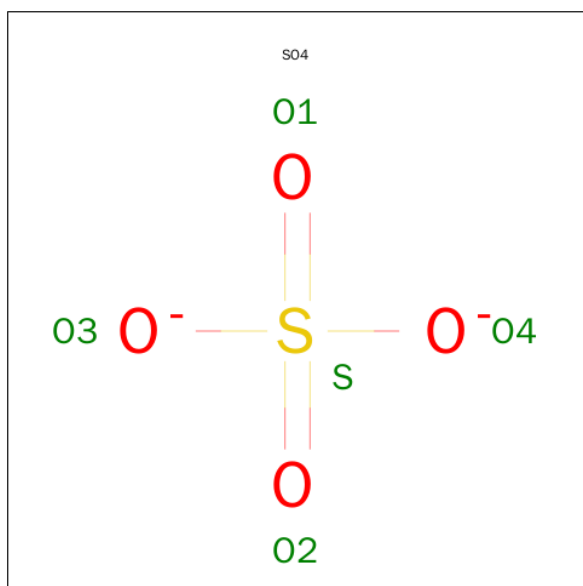
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	2	Total	C	N	O	0	0
			28	16	2	10		
6	B	2	Total	C	N	O	0	0
			28	16	2	10		
6	B	2	Total	C	N	O	0	0
			28	16	2	10		

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

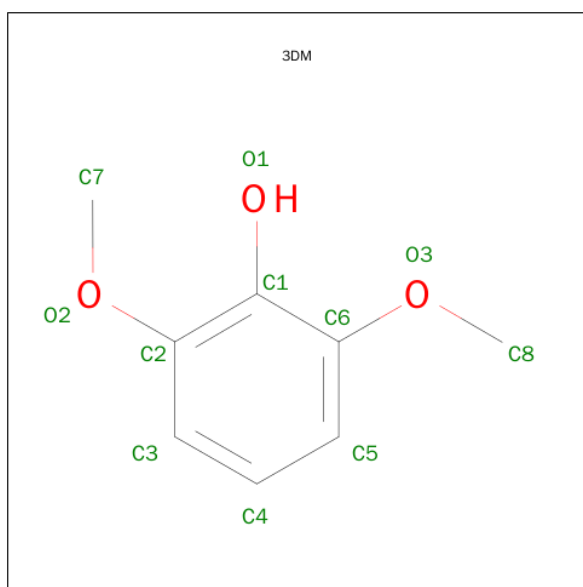
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	3	Total	C	N	O	0	0
			39	22	2	15		
7	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



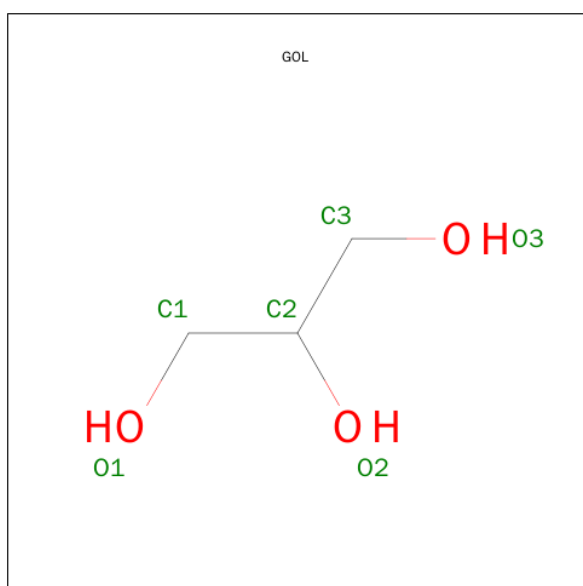
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is 2,6-DIMETHOXYPHENOL (three-letter code: 3DM) (formula: C₈H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			11	8	3		
9	B	1	Total	C	O	0	0
			11	8	3		

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	1
			6	3	3		
10	B	1	Total	C	O	0	1
			6	3	3		

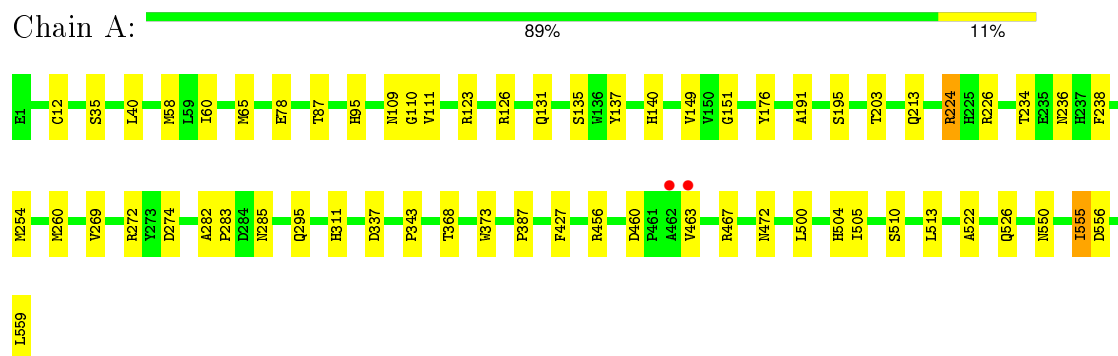
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	677	Total 677	O 677	0	0
11	B	659	Total 659	O 659	0	0

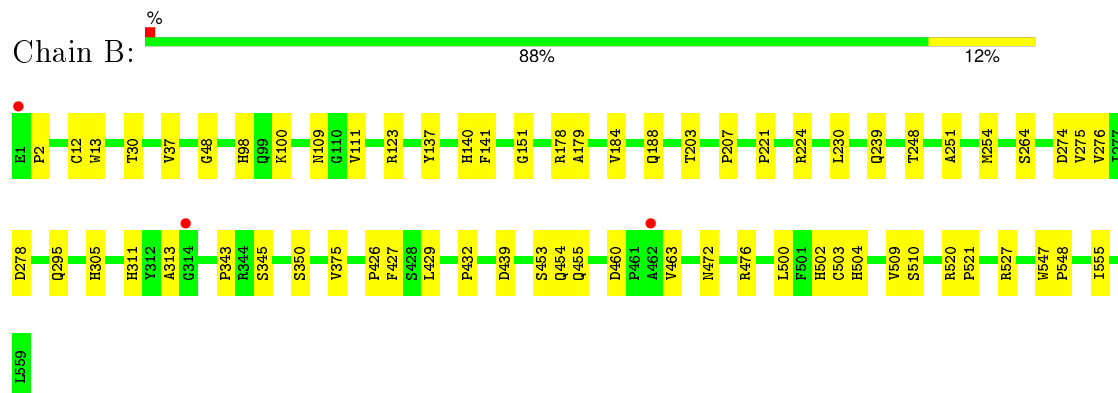
3 Residue-property plots

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: Laccase-1



• Molecule 1: Laccase-1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	174.71Å 62.37Å 125.14Å 90.00° 96.36° 90.00°	Depositor
Resolution (Å)	19.78 – 1.80 19.78 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.78-1.80) 98.8 (19.78-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.203 , 0.256 0.204 , 0.255	Depositor DCC
R_{free} test set	6134 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	15.7	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 62.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 122679 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10570	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.56% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, CL, OHI, SO4, 3DM, CU, MAN

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	0.76	0/4518	0.77	0/6205
1	B	0.76	0/4517	0.76	0/6203
All	All	0.76	0/9035	0.76	0/12408

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
5	A	1	0
5	B	1	0
7	A	1	0
7	B	1	0
All	All	4	0

There are no bond length outliers.

There are no bond angle outliers.

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	712	MAN	C1
7	A	732	MAN	C1
5	B	712	MAN	C1
7	B	732	MAN	C1

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	4394	0	4124	50	0
1	B	4393	0	4126	42	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	28	0	26	0	0
4	B	42	0	39	1	0
5	A	50	0	43	0	0
5	B	50	0	42	1	0
6	A	84	0	75	1	0
6	B	56	0	50	1	0
7	A	39	0	34	0	0
7	B	39	0	34	0	0
8	A	10	0	0	0	0
8	B	5	0	0	0	0
9	A	11	0	9	2	0
9	B	11	0	9	0	0
10	A	6	0	4	1	0
10	B	6	0	4	0	0
11	A	677	0	0	23	0
11	B	659	0	0	26	0
All	All	10570	0	8619	93	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.

The worst 5 of 93 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:B:141:PHE:HB2	11:B:1255:HOH:O	1.23	1.25
1:A:224:ARG:HH11	1:A:224:ARG:HG3	1.21	1.03
1:A:295:GLN:HG3	11:A:1247:HOH:O	1.59	1.02
1:A:337:ASP:HB2	11:A:1103:HOH:O	1.61	1.00
1:B:275:VAL:HB	11:B:1094:HOH:O	1.68	0.92

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	560/559 (100%)	545 (97%)	15 (3%)	0	100	100
1	B	559/559 (100%)	546 (98%)	13 (2%)	0	100	100
All	All	1119/1118 (100%)	1091 (98%)	28 (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	481/477 (101%)	471 (98%)	10 (2%)	61	47
1	B	480/477 (101%)	469 (98%)	11 (2%)	58	42
All	All	961/954 (101%)	940 (98%)	21 (2%)	63	45

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	555	ILE
1	B	12[B]	CYS
1	B	345	SER
1	A	513	LEU
1	B	350	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	550	ASN
1	B	455	GLN
1	B	99	GLN
1	A	455	GLN
1	B	68	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	OHI	A	98	1	10,11,12	1.39	1 (10%)	4,14,16	2.28	2 (50%)
1	OHI	B	98	1	10,11,12	0.99	0	4,14,16	2.16	2 (50%)

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
1	OHI	A	98	1	-	0/2/15/17	0/1/1/1
1	OHI	B	98	1	-	0/2/15/17	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	OHI	O12-CE1	2.97	1.29	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	OHI	CA-CB-CG	-3.41	107.32	114.45
1	B	98	OHI	CA-CB-CG	-3.01	108.16	114.45
1	B	98	OHI	O-C-CA	-3.00	117.69	125.49
1	A	98	OHI	O-C-CA	-2.99	117.70	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	98	OHI	1	0

5.5 Carbohydrates ⓘ

24 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	$\# Z > 2$
5	NAG	A	710	1,5	14,14,15	0.69	0	15,19,21	1.35	1 (6%)
5	NAG	A	711	5	14,14,15	0.68	0	15,19,21	1.57	3 (20%)
5	MAN	A	712	5	11,11,12	0.84	1 (9%)	14,15,17	1.94	4 (28%)
5	MAN	A	714	5	11,11,12	0.77	1 (9%)	14,15,17	1.28	2 (14%)
6	NAG	A	720	1,6	14,14,15	0.65	0	15,19,21	1.07	1 (6%)
6	NAG	A	721	6	14,14,15	0.61	0	15,19,21	1.26	2 (13%)
7	NAG	A	730	1,7	14,14,15	0.71	0	15,19,21	1.00	0
7	NAG	A	731	7	14,14,15	0.63	0	15,19,21	0.89	0
7	MAN	A	732	7	11,11,12	0.66	0	14,15,17	1.48	3 (21%)
6	NAG	A	740	1,6	14,14,15	0.60	0	15,19,21	1.54	1 (6%)
6	NAG	A	741	6	14,14,15	0.51	0	15,19,21	1.85	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	760	1,6	14,14,15	0.85	1 (7%)	15,19,21	0.89	0
6	NAG	A	761	6	14,14,15	0.61	0	15,19,21	2.10	5 (33%)
5	NAG	B	710	1,5	14,14,15	0.75	0	15,19,21	1.10	1 (6%)
5	NAG	B	711	5	14,14,15	0.64	0	15,19,21	1.36	2 (13%)
5	MAN	B	712	5	11,11,12	0.68	0	14,15,17	1.94	3 (21%)
5	MAN	B	714	5	11,11,12	0.69	0	14,15,17	1.34	2 (14%)
6	NAG	B	720	1,6	14,14,15	0.60	0	15,19,21	1.00	1 (6%)
6	NAG	B	721	6	14,14,15	0.65	0	15,19,21	1.32	3 (20%)
7	NAG	B	730	1,7	14,14,15	0.61	0	15,19,21	1.34	3 (20%)
7	NAG	B	731	7	14,14,15	0.73	0	15,19,21	1.02	0
7	MAN	B	732	7	11,11,12	0.55	0	14,15,17	1.43	2 (14%)
6	NAG	B	740	1,6	14,14,15	0.51	0	15,19,21	1.44	3 (20%)
6	NAG	B	741	6	14,14,15	0.58	0	15,19,21	1.20	1 (6%)

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
5	NAG	A	710	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	711	5	-	0/6/23/26	0/1/1/1
5	MAN	A	712	5	1/1/4/5	0/2/19/22	0/1/1/1
5	MAN	A	714	5	-	0/2/19/22	0/1/1/1
6	NAG	A	720	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	721	6	-	0/6/23/26	0/1/1/1
7	NAG	A	730	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	731	7	-	0/6/23/26	0/1/1/1
7	MAN	A	732	7	1/1/4/5	0/2/19/22	0/1/1/1
6	NAG	A	740	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	741	6	-	0/6/23/26	0/1/1/1
6	NAG	A	760	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	761	6	-	0/6/23/26	0/1/1/1
5	NAG	B	710	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	711	5	-	0/6/23/26	0/1/1/1
5	MAN	B	712	5	1/1/4/5	0/2/19/22	0/1/1/1
5	MAN	B	714	5	-	0/2/19/22	0/1/1/1
6	NAG	B	720	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	721	6	-	0/6/23/26	0/1/1/1
7	NAG	B	730	1,7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	731	7	-	0/6/23/26	0/1/1/1
7	MAN	B	732	7	1/1/4/5	0/2/19/22	0/1/1/1
6	NAG	B	740	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	741	6	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	760	NAG	O5-C1	-2.52	1.39	1.43
5	A	712	MAN	O5-C1	-2.01	1.40	1.43
5	A	714	MAN	C2-C3	2.17	1.55	1.52

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	712	MAN	C1-O5-C5	-4.63	106.38	112.25
6	A	741	NAG	C2-N2-C7	-4.35	117.44	123.04
6	A	761	NAG	C3-C4-C5	-3.84	103.50	110.20
5	A	712	MAN	O5-C1-C2	-3.64	104.95	110.86
5	B	712	MAN	C3-C4-C5	-3.19	104.63	110.20

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	712	MAN	C1
7	A	732	MAN	C1
7	B	732	MAN	C1
5	A	712	MAN	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	721	NAG	1	0
5	B	711	NAG	1	0
6	B	720	NAG	1	0

5.6 Ligand geometry

Of 22 ligands modelled in this entry, 10 are monoatomic - leaving 12 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$
9	3DM	A	2900	-	11,11,11	3.12	2 (18%)	14,14,14	2.79	6 (42%)
8	SO4	A	3800	-	4,4,4	0.26	0	6,6,6	0.72	0
8	SO4	A	3801	-	4,4,4	0.17	0	6,6,6	0.28	0
10	GOL	A	3902[A]	-	5,5,5	0.31	0	5,5,5	0.53	0
4	NAG	A	700	1	14,14,15	0.83	1 (7%)	15,19,21	1.85	3 (20%)
4	NAG	A	750	1	14,14,15	0.64	0	15,19,21	1.21	2 (13%)
4	NAG	B	1750	1	14,14,15	0.67	0	15,19,21	1.65	2 (13%)
4	NAG	B	2760	1	14,14,15	0.75	1 (7%)	15,19,21	0.79	0
9	3DM	B	2910	-	11,11,11	2.88	2 (18%)	14,14,14	2.25	4 (28%)
10	GOL	B	3901[B]	-	5,5,5	0.32	0	5,5,5	0.40	0
8	SO4	B	4802	-	4,4,4	0.19	0	6,6,6	0.27	0
4	NAG	B	700	1	14,14,15	0.59	0	15,19,21	1.09	1 (6%)

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
9	3DM	A	2900	-	-	0/4/4/4	0/1/1/1
8	SO4	A	3800	-	-	0/0/0/0	0/0/0/0
8	SO4	A	3801	-	-	0/0/0/0	0/0/0/0
10	GOL	A	3902[A]	-	-	0/4/4/4	0/0/0/0
4	NAG	A	700	1	-	0/6/23/26	0/1/1/1
4	NAG	A	750	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1750	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2760	1	-	0/6/23/26	0/1/1/1
9	3DM	B	2910	-	-	0/4/4/4	0/1/1/1
10	GOL	B	3901[B]	-	-	0/4/4/4	0/0/0/0
8	SO4	B	4802	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	700	1	-	0/6/23/26	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	700	NAG	C1-C2	2.20	1.55	1.52
4	B	2760	NAG	C1-C2	2.46	1.55	1.52
9	B	2910	3DM	C2-C1	6.29	1.48	1.40
9	A	2900	3DM	C2-C1	6.64	1.49	1.40
9	B	2910	3DM	C6-C1	6.85	1.49	1.40

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	700	NAG	C3-C2-N2	-3.98	101.04	110.56
9	A	2900	3DM	O3-C6-C5	-2.49	120.17	124.35
4	A	750	NAG	C4-C3-C2	-2.21	107.79	111.23
9	A	2900	3DM	O2-C2-C3	-2.08	120.85	124.35
4	A	700	NAG	C6-C5-C4	-2.07	107.91	113.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2900	3DM	2	0
10	A	3902[A]	GOL	1	0
4	B	1750	NAG	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 ⓘ

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	558/559 (99%)	-0.23	2 (0%) 93 91	9, 16, 26, 40	0
1	B	558/559 (99%)	-0.14	3 (0%) 91 90	9, 17, 27, 38	0
All	All	1116/1118 (99%)	-0.19	5 (0%) 93 91	9, 17, 27, 40	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	GLU	3.3
1	A	463	VAL	3.1
1	B	462	ALA	2.8
1	B	314	GLY	2.2
1	A	462	ALA	2.0

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

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
1	OHI	B	98	11/12	0.89	0.12	-	15,18,27,31	0
1	OHI	A	98	11/12	0.89	0.12	-	16,19,25,26	0

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, 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	NAG	A	760	14/15	0.81	0.17	4.77	24,30,33,36	0
6	NAG	A	720	14/15	0.85	0.15	2.92	25,27,31,34	0
6	NAG	B	720	14/15	0.82	0.17	1.87	30,32,34,34	0
6	NAG	B	721	14/15	0.79	0.21	1.78	28,37,38,39	0
5	NAG	B	711	14/15	0.93	0.10	1.20	13,21,31,32	0
7	NAG	A	731	14/15	0.92	0.12	1.04	21,27,29,33	0
6	NAG	A	721	14/15	0.88	0.14	0.95	24,31,33,34	0
6	NAG	B	740	14/15	0.88	0.11	0.74	17,21,28,29	0
7	NAG	B	731	14/15	0.90	0.14	0.51	24,29,33,36	0
6	NAG	A	740	14/15	0.89	0.12	0.39	17,19,26,29	0
5	NAG	A	711	14/15	0.94	0.12	0.12	13,18,23,26	0
7	NAG	A	730	14/15	0.95	0.08	-0.33	15,19,21,21	0
5	NAG	A	710	14/15	0.96	0.07	-1.59	10,12,14,14	0
7	NAG	B	730	14/15	0.97	0.07	-1.87	17,20,24,24	0
5	NAG	B	710	14/15	0.97	0.07	-2.17	11,13,16,18	0
6	NAG	B	741	14/15	0.83	0.26	-	33,37,41,41	0
6	NAG	A	741	14/15	0.86	0.24	-	31,35,40,40	0
6	NAG	A	761	14/15	0.85	0.33	-	40,44,46,47	0
5	MAN	A	714	11/12	0.74	0.27	-	32,36,37,40	0
5	MAN	B	712	11/12	0.82	0.17	-	34,39,42,43	0
5	MAN	A	712	11/12	0.74	0.23	-	28,32,35,38	0
5	MAN	B	714	11/12	0.75	0.30	-	40,45,49,52	0
7	MAN	A	732	11/12	0.76	0.24	-	39,43,45,48	0
7	MAN	B	732	11/12	0.69	0.31	-	41,45,46,46	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(Å ²)	Q<0.9
9	3DM	A	2900	11/11	0.71	0.22	8.45	37,40,42,44	0
4	NAG	A	700	14/15	0.85	0.17	7.96	23,27,31,35	0
4	NAG	B	2760	14/15	0.80	0.16	5.12	23,29,32,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	3DM	B	2910	11/11	0.70	0.20	4.50	43,46,46,46	0
10	GOL	A	3902[A]	6/6	0.79	0.23	4.09	31,32,33,33	6
4	NAG	A	750	14/15	0.83	0.21	3.56	33,38,41,43	0
4	NAG	B	700	14/15	0.88	0.15	2.99	25,27,34,35	0
4	NAG	B	1750	14/15	0.89	0.12	1.60	23,25,29,29	0
3	CL	B	610	1/1	0.98	0.10	0.48	24,24,24,24	0
8	SO4	A	3801	5/5	0.91	0.12	-0.16	44,44,46,47	0
3	CL	A	610	1/1	0.99	0.07	-0.31	22,22,22,22	0
2	CU	B	604	1/1	1.00	0.02	-2.77	17,17,17,17	0
2	CU	A	601	1/1	1.00	0.04	-3.20	14,14,14,14	0
2	CU	B	603	1/1	1.00	0.01	-3.62	13,13,13,13	0
2	CU	A	603	1/1	1.00	0.04	-4.74	13,13,13,13	0
2	CU	B	601	1/1	1.00	0.03	-5.21	14,14,14,14	0
2	CU	B	602	1/1	1.00	0.01	-5.38	17,17,17,17	0
2	CU	A	602	1/1	1.00	0.02	-9.09	16,16,16,16	0
2	CU	A	604	1/1	1.00	0.01	-10.10	17,17,17,17	0
10	GOL	B	3901[B]	6/6	0.76	0.24	-	25,26,27,27	6
8	SO4	A	3800	5/5	0.93	0.11	-	44,46,47,47	0
8	SO4	B	4802	5/5	0.92	0.09	-	53,54,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.