



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:45 AM GMT

PDB ID : 3PPS
Title : Crystal structure of an ascomycete fungal laccase from Thielavia arenaria
Authors : Kallio, J.P.; Rouvinen, J.; Hakulinen, N.
Deposited on : 2010-11-25
Resolution : 2.50 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

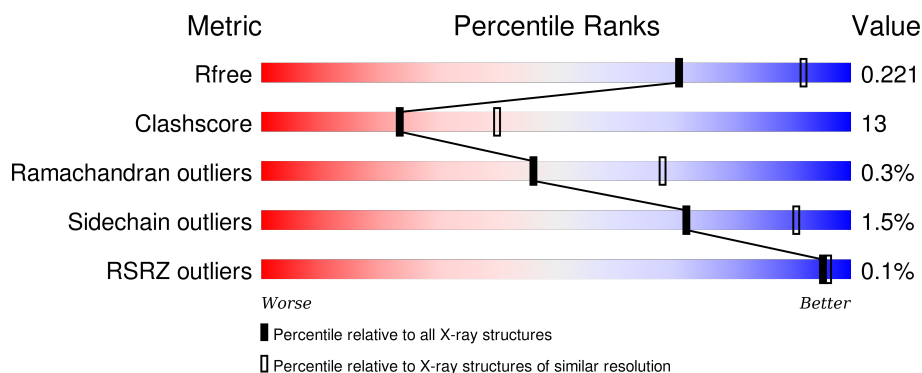
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 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	604	
1	B	604	
1	C	604	
1	D	604	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 18812 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.

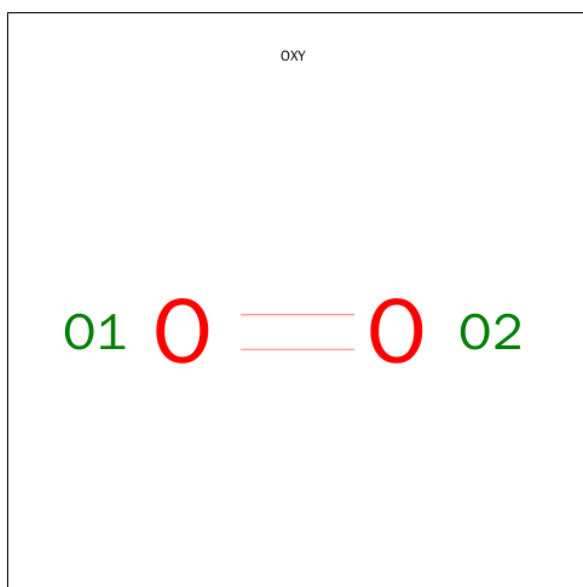
- Molecule 1 is a protein called Laccase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	564	Total	C	N	O	S	0	0	0
			4406	2793	776	821	16			
1	B	564	Total	C	N	O	S	0	0	0
			4406	2793	776	821	16			
1	C	564	Total	C	N	O	S	0	0	0
			4406	2793	776	821	16			
1	D	564	Total	C	N	O	S	0	0	0
			4406	2793	776	821	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		
2	D	4	Total	Cu	0	0
			4	4		
2	C	4	Total	Cu	0	0
			4	4		

- Molecule 3 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O₂).



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

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 5 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	5	Total	C	N	O	0	0
			61	34	2	25		
7	D	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 8 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	3	Total	C	N	O	0	0
			39	22	2	15		
8	D	3	Total	C	N	O	0	0
			39	22	2	15		

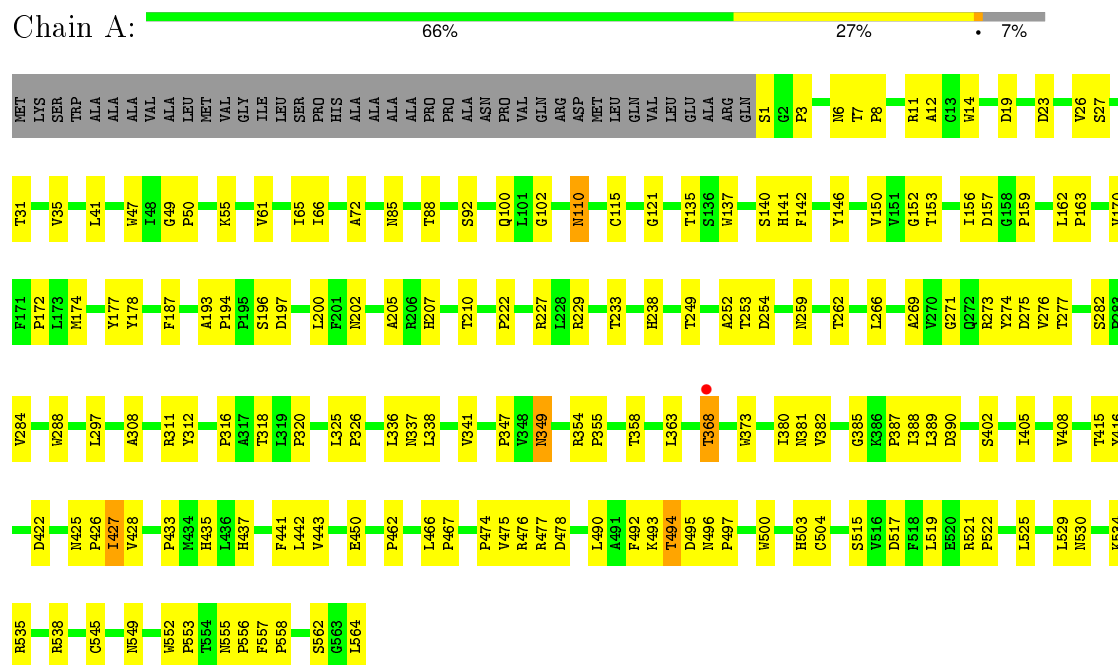
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	159	Total	O	0	0
			159	159		
9	B	138	Total	O	0	0
			138	138		
9	C	124	Total	O	0	0
			124	124		
9	D	141	Total	O	0	0
			141	141		

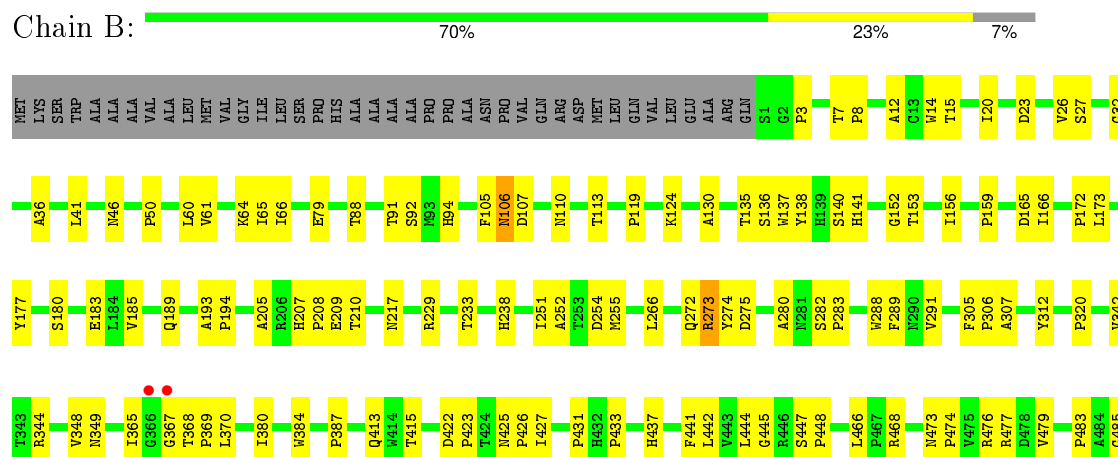
3 Residue-property plots

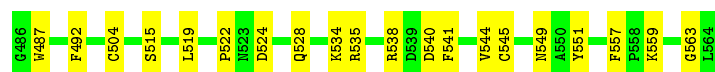
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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



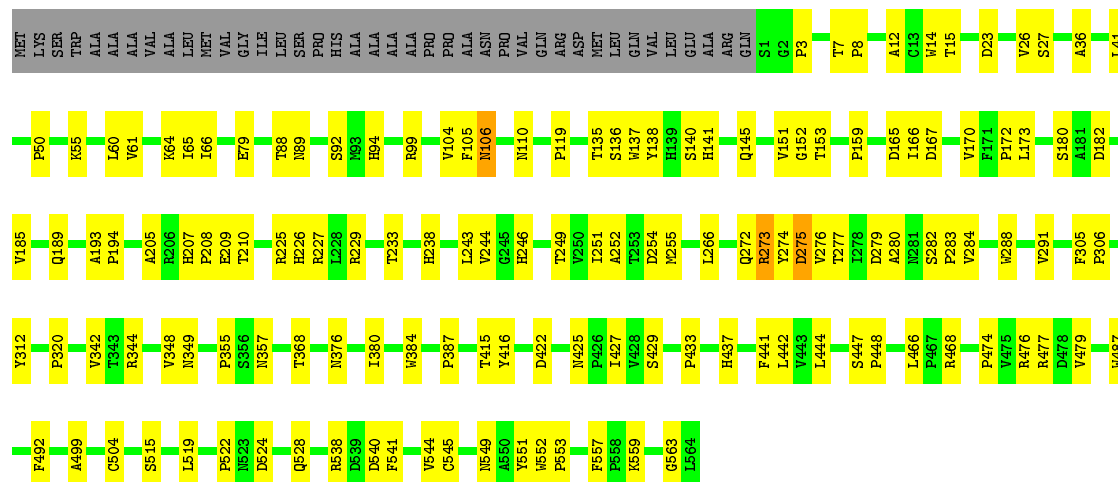
• Molecule 1: Laccase





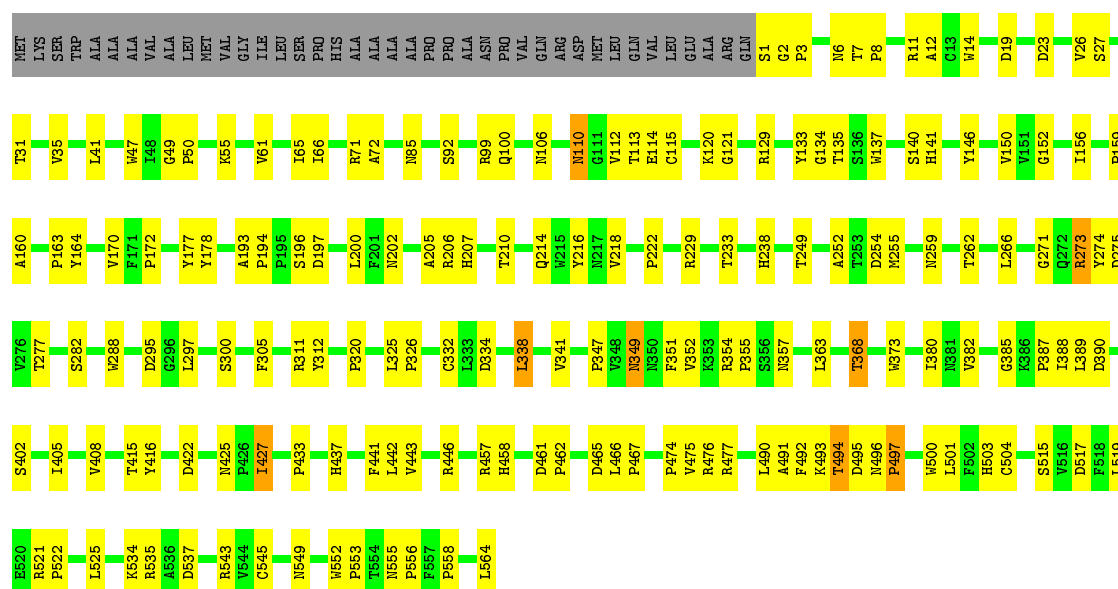
• Molecule 1: Laccase

Chain C: 70% 23% 7%



• Molecule 1: Laccase

Chain D: 65% 27% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.36Å 178.95Å 118.13Å 90.00° 90.26° 90.00°	Depositor
Resolution (Å)	42.65 – 2.50 42.65 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.65-2.50) 98.6 (42.65-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.182 , 0.222 0.179 , 0.221	Depositor DCC
R_{free} test set	4405 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	12.6	Xtriage
Anisotropy	1.837	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 7.9	EDS
Estimated twinning fraction	0.319 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 87766 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	18812	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.22 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.4366e-04.*

¹ Intensities estimated from amplitudes.

² 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, BMA, NAG, CU, OXY

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	0.36	0/4539	0.53	0/6219
1	B	0.36	0/4539	0.53	0/6219
1	C	0.35	0/4539	0.53	0/6219
1	D	0.35	0/4539	0.53	0/6219
All	All	0.35	0/18156	0.53	0/24876

There are no bond length outliers.

There are no bond angle outliers.

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	4406	0	4223	129	0
1	B	4406	0	4223	105	0
1	C	4406	0	4224	103	0
1	D	4406	0	4225	136	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
3	A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	56	0	50	4	0
4	B	56	0	50	2	0
4	C	84	0	75	9	0
4	D	28	0	25	0	0
5	A	72	0	61	1	0
6	A	42	0	39	1	0
6	B	42	0	39	0	0
6	C	14	0	13	0	0
6	D	14	0	13	1	0
7	B	61	0	52	2	0
7	D	61	0	52	4	0
8	C	39	0	34	3	0
8	D	39	0	34	1	0
9	A	159	0	0	12	0
9	B	138	0	0	15	0
9	C	124	0	0	14	0
9	D	141	0	0	28	0
All	All	18812	0	17432	473	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 13.

The worst 5 of 473 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:C:376:ASN:HD22	4:C:760:NAG:H83	1.35	0.92
1:A:253:THR:HG21	1:A:338:LEU:HD12	1.59	0.83
1:D:207:HIS:HD2	1:D:210:THR:H	1.27	0.82
1:A:207:HIS:HD2	1:A:210:THR:H	1.28	0.81
1:C:104:VAL:HG11	9:C:694:HOH:O	1.79	0.81

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	562/604 (93%)	517 (92%)	42 (8%)	3 (0%)	34	55
1	B	562/604 (93%)	502 (89%)	60 (11%)	0	100	100
1	C	562/604 (93%)	505 (90%)	57 (10%)	0	100	100
1	D	562/604 (93%)	515 (92%)	44 (8%)	3 (0%)	34	55
All	All	2248/2416 (93%)	2039 (91%)	203 (9%)	6 (0%)	46	68

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	494	THR
1	D	494	THR
1	A	284	VAL
1	D	222	PRO
1	D	497	PRO

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	484/513 (94%)	477 (99%)	7 (1%)	74	91
1	B	484/513 (94%)	476 (98%)	8 (2%)	68	89
1	C	484/513 (94%)	477 (99%)	7 (1%)	74	91
1	D	484/513 (94%)	476 (98%)	8 (2%)	68	89
All	All	1936/2052 (94%)	1906 (98%)	30 (2%)	72	91

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	349	ASN
1	C	110	ASN
1	D	349	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	106	ASN
1	C	141	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	240	GLN
1	C	10	ASN
1	C	240	GLN
1	B	207	HIS
1	D	103	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 ⓘ

38 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	$\# Z > 2$
4	NAG	A	700	1,4	14,14,15	0.49	0	15,19,21	1.79	4 (26%)
4	NAG	A	701	4	14,14,15	0.41	0	15,19,21	1.61	1 (6%)
5	NAG	A	710	1,5	14,14,15	0.54	0	15,19,21	0.94	0
5	NAG	A	711	5	14,14,15	0.59	0	15,19,21	1.17	2 (13%)
5	BMA	A	712	5	11,11,12	0.50	0	14,15,17	1.22	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	A	713	5	11,11,12	0.44	0	14,15,17	0.91	1 (7%)
5	MAN	A	714	5	11,11,12	0.82	1 (9%)	14,15,17	1.47	3 (21%)
5	MAN	A	715	5	11,11,12	0.90	0	14,15,17	2.00	5 (35%)
4	NAG	A	740	1,4	14,14,15	0.65	0	15,19,21	1.31	3 (20%)
4	NAG	A	741	4	14,14,15	0.53	0	15,19,21	1.06	1 (6%)
4	NAG	B	700	1,4	14,14,15	0.51	0	15,19,21	1.58	2 (13%)
4	NAG	B	701	4	14,14,15	0.49	0	15,19,21	1.38	2 (13%)
7	NAG	B	710	1,7	14,14,15	0.71	0	15,19,21	1.02	1 (6%)
7	NAG	B	711	7	14,14,15	0.63	0	15,19,21	0.99	0
7	BMA	B	712	7	11,11,12	0.67	0	14,15,17	0.96	0
7	MAN	B	714	7	11,11,12	0.65	0	14,15,17	1.41	2 (14%)
7	MAN	B	715	7	11,11,12	0.49	0	14,15,17	1.75	5 (35%)
4	NAG	B	740	1,4	14,14,15	0.43	0	15,19,21	0.90	0
4	NAG	B	741	4	14,14,15	0.54	0	15,19,21	0.90	0
4	NAG	C	700	1,4	14,14,15	0.42	0	15,19,21	1.16	1 (6%)
4	NAG	C	701	4	14,14,15	0.50	0	15,19,21	0.80	0
8	NAG	C	710	1,8	14,14,15	0.54	0	15,19,21	0.76	0
8	NAG	C	711	8	14,14,15	0.41	0	15,19,21	1.37	1 (6%)
8	BMA	C	712	8	11,11,12	0.77	0	14,15,17	1.24	2 (14%)
4	NAG	C	740	1,4	14,14,15	0.64	0	15,19,21	1.33	1 (6%)
4	NAG	C	741	4	14,14,15	0.40	0	15,19,21	1.96	3 (20%)
4	NAG	C	760	1,4	14,14,15	0.51	0	15,19,21	1.29	2 (13%)
4	NAG	C	761	4	14,14,15	0.57	0	15,19,21	0.89	1 (6%)
8	NAG	D	700	1,8	14,14,15	0.45	0	15,19,21	1.60	1 (6%)
8	NAG	D	701	8	14,14,15	0.51	0	15,19,21	1.02	1 (6%)
8	BMA	D	702	8	11,11,12	0.59	0	14,15,17	0.75	1 (7%)
7	NAG	D	710	1,7	14,14,15	0.48	0	15,19,21	1.60	2 (13%)
7	NAG	D	711	7	14,14,15	0.69	0	15,19,21	1.69	3 (20%)
7	BMA	D	712	7	11,11,12	0.66	0	14,15,17	0.95	1 (7%)
7	MAN	D	714	7	11,11,12	0.73	0	14,15,17	1.74	5 (35%)
7	MAN	D	715	7	11,11,12	0.62	0	14,15,17	1.28	3 (21%)
4	NAG	D	740	1,4	14,14,15	0.51	0	15,19,21	1.31	1 (6%)
4	NAG	D	741	4	14,14,15	0.39	0	15,19,21	1.45	2 (13%)

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. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	700	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	701	4	-	0/6/23/26	0/1/1/1
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	BMA	A	712	5	-	0/2/19/22	0/1/1/1
5	MAN	A	713	5	-	0/2/19/22	0/1/1/1
5	MAN	A	714	5	-	0/2/19/22	0/1/1/1
5	MAN	A	715	5	-	0/2/19/22	0/1/1/1
4	NAG	A	740	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	741	4	-	0/6/23/26	0/1/1/1
4	NAG	B	700	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	701	4	-	0/6/23/26	0/1/1/1
7	NAG	B	710	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	711	7	-	0/6/23/26	0/1/1/1
7	BMA	B	712	7	-	0/2/19/22	0/1/1/1
7	MAN	B	714	7	-	0/2/19/22	0/1/1/1
7	MAN	B	715	7	-	0/2/19/22	0/1/1/1
4	NAG	B	740	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	741	4	-	0/6/23/26	0/1/1/1
4	NAG	C	700	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	701	4	-	0/6/23/26	0/1/1/1
8	NAG	C	710	1,8	-	0/6/23/26	0/1/1/1
8	NAG	C	711	8	-	0/6/23/26	0/1/1/1
8	BMA	C	712	8	-	0/2/19/22	0/1/1/1
4	NAG	C	740	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	741	4	-	0/6/23/26	0/1/1/1
4	NAG	C	760	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	761	4	-	0/6/23/26	0/1/1/1
8	NAG	D	700	1,8	-	0/6/23/26	0/1/1/1
8	NAG	D	701	8	-	0/6/23/26	0/1/1/1
8	BMA	D	702	8	-	0/2/19/22	0/1/1/1
7	NAG	D	710	1,7	-	0/6/23/26	0/1/1/1
7	NAG	D	711	7	-	0/6/23/26	0/1/1/1
7	BMA	D	712	7	-	0/2/19/22	0/1/1/1
7	MAN	D	714	7	-	0/2/19/22	0/1/1/1
7	MAN	D	715	7	-	0/2/19/22	0/1/1/1
4	NAG	D	740	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	741	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	714	MAN	O5-C1	-2.07	1.40	1.43

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	711	NAG	C2-N2-C7	-4.49	117.28	123.04
5	A	715	MAN	C2-C3-C4	-4.15	103.99	111.04
4	C	760	NAG	C2-N2-C7	-3.98	117.92	123.04
4	C	741	NAG	C4-C3-C2	-3.74	105.42	111.23
7	D	710	NAG	C2-N2-C7	-3.71	118.28	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	700	NAG	3	0
4	A	701	NAG	1	0
5	A	711	NAG	1	0
7	B	710	NAG	1	0
7	B	711	NAG	1	0
7	B	714	MAN	1	0
4	B	740	NAG	1	0
4	B	741	NAG	2	0
4	C	701	NAG	4	0
8	C	710	NAG	1	0
8	C	711	NAG	2	0
8	C	712	BMA	1	0
4	C	741	NAG	1	0
4	C	760	NAG	3	0
4	C	761	NAG	1	0
8	D	700	NAG	1	0
7	D	710	NAG	3	0
7	D	711	NAG	1	0

5.6 Ligand geometry

Of 25 ligands modelled in this entry, 16 are monoatomic - leaving 9 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
3	OXY	A	620	2	1,1,1	0.31	0	0,0,0	0.00	-
6	NAG	A	720	1	14,14,15	0.56	0	15,19,21	0.84	1 (6%)
6	NAG	A	730	1	14,14,15	0.58	0	15,19,21	1.38	1 (6%)
6	NAG	A	760	1	14,14,15	0.62	0	15,19,21	1.43	2 (13%)
6	NAG	B	720	1	14,14,15	0.51	0	15,19,21	1.06	1 (6%)
6	NAG	B	760	1	14,14,15	0.55	0	15,19,21	1.71	2 (13%)
6	NAG	B	770	1	14,14,15	0.56	0	15,19,21	1.28	3 (20%)
6	NAG	C	730	1	14,14,15	0.46	0	15,19,21	1.68	2 (13%)
6	NAG	D	720	1	14,14,15	0.51	0	15,19,21	1.44	2 (13%)

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
3	OXY	A	620	2	-	0/0/0/0	0/0/0/0
6	NAG	A	720	1	-	0/6/23/26	0/1/1/1
6	NAG	A	730	1	-	0/6/23/26	0/1/1/1
6	NAG	A	760	1	-	0/6/23/26	0/1/1/1
6	NAG	B	720	1	-	0/6/23/26	0/1/1/1
6	NAG	B	760	1	-	0/6/23/26	0/1/1/1
6	NAG	B	770	1	-	1/6/23/26	0/1/1/1
6	NAG	C	730	1	-	0/6/23/26	0/1/1/1
6	NAG	D	720	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	760	NAG	C2-N2-C7	-4.57	117.17	123.04
6	B	760	NAG	C2-N2-C7	-4.56	117.18	123.04
6	C	730	NAG	C4-C3-C2	-3.36	106.01	111.23
6	B	770	NAG	C1-O5-C5	-3.08	108.34	112.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	760	NAG	C1-O5-C5	-2.10	109.58	112.25

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	770	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	760	NAG	1	0
6	D	720	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 [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	564/604 (93%)	-0.58	1 (0%) 95 96	11, 19, 31, 50	0
1	B	564/604 (93%)	-0.62	2 (0%) 93 93	9, 19, 34, 47	0
1	C	564/604 (93%)	-0.62	0 100 100	10, 20, 34, 48	0
1	D	564/604 (93%)	-0.48	0 100 100	11, 20, 32, 51	0
All	All	2256/2416 (93%)	-0.58	3 (0%) 95 96	9, 19, 33, 51	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	368	THR	3.6
1	B	367	GLY	2.6
1	B	366	GLY	2.1

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
8	NAG	D	701	14/15	0.96	0.14	1.03	15,26,42,54	0
4	NAG	C	741	14/15	0.93	0.14	0.64	12,24,29,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	NAG	A	711	14/15	0.95	0.13	0.50	7,18,25,28	0
8	NAG	C	710	14/15	0.95	0.13	0.47	12,20,29,29	0
4	NAG	B	700	14/15	0.94	0.13	0.36	8,16,23,26	0
4	NAG	C	760	14/15	0.94	0.12	0.33	8,27,36,45	0
7	NAG	B	711	14/15	0.96	0.12	0.13	8,22,28,30	0
8	NAG	C	711	14/15	0.96	0.12	0.04	19,25,33,38	0
4	NAG	D	740	14/15	0.94	0.12	-0.06	12,23,34,35	0
4	NAG	A	701	14/15	0.95	0.11	-0.23	12,19,29,30	0
4	NAG	C	701	14/15	0.94	0.12	-0.31	14,28,40,40	0
4	NAG	B	701	14/15	0.96	0.11	-0.34	10,14,25,26	0
4	NAG	B	740	14/15	0.96	0.10	-0.49	8,24,32,34	0
4	NAG	C	740	14/15	0.97	0.11	-0.56	13,23,30,36	0
7	NAG	B	710	14/15	0.97	0.10	-0.62	12,19,27,34	0
5	NAG	A	710	14/15	0.97	0.10	-0.70	11,15,24,25	0
4	NAG	A	740	14/15	0.97	0.10	-0.81	11,16,25,28	0
8	NAG	D	700	14/15	0.97	0.10	-1.06	13,18,25,25	0
7	NAG	D	710	14/15	0.97	0.10	-1.30	17,28,32,33	0
4	NAG	A	700	14/15	0.98	0.10	-1.49	9,16,22,30	0
4	NAG	C	700	14/15	0.97	0.09	-1.80	12,20,28,29	0
5	MAN	A	713	11/12	0.90	0.21	-	16,32,37,42	0
7	NAG	D	711	14/15	0.95	0.13	-	21,28,39,44	0
5	MAN	A	714	11/12	0.95	0.13	-	17,24,33,39	0
7	MAN	B	715	11/12	0.91	0.15	-	18,29,36,38	0
4	NAG	B	741	14/15	0.95	0.14	-	17,28,33,34	0
8	BMA	C	712	11/12	0.92	0.14	-	12,28,36,37	0
5	BMA	A	712	11/12	0.96	0.12	-	12,25,33,34	0
7	MAN	D	715	11/12	0.85	0.16	-	32,50,60,63	0
5	MAN	A	715	11/12	0.87	0.17	-	18,26,37,41	0
4	NAG	D	741	14/15	0.93	0.13	-	16,36,42,44	0
8	BMA	D	702	11/12	0.82	0.19	-	38,51,61,65	0
4	NAG	A	741	14/15	0.96	0.14	-	19,25,31,35	0
7	BMA	B	712	11/12	0.96	0.11	-	9,24,28,40	0
4	NAG	C	761	14/15	0.89	0.24	-	18,33,42,48	0
7	MAN	D	714	11/12	0.90	0.18	-	24,41,53,54	0
7	MAN	B	714	11/12	0.94	0.10	-	16,30,35,37	0
7	BMA	D	712	11/12	0.94	0.12	-	32,48,57,68	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
6	NAG	A	760	14/15	0.96	0.14	1.28	12,21,25,30	0
6	NAG	B	760	14/15	0.96	0.12	0.34	6,15,25,28	0
6	NAG	B	720	14/15	0.94	0.14	0.20	13,23,35,36	0
6	NAG	D	720	14/15	0.94	0.14	0.06	14,20,28,32	0
2	CU	D	602	1/1	1.00	0.09	-0.36	26,26,26,26	0
3	OXY	A	620	2/2	0.99	0.10	-1.90	5,5,5,8	0
2	CU	C	603	1/1	1.00	0.09	-1.98	18,18,18,18	0
2	CU	B	602	1/1	1.00	0.08	-2.27	17,17,17,17	0
2	CU	D	603	1/1	0.99	0.06	-2.62	20,20,20,20	0
2	CU	B	603	1/1	1.00	0.07	-2.64	13,13,13,13	0
2	CU	C	601	1/1	1.00	0.07	-2.75	21,21,21,21	0
2	CU	A	601	1/1	0.99	0.07	-3.05	31,31,31,31	0
2	CU	B	601	1/1	0.99	0.06	-3.13	21,21,21,21	0
2	CU	D	604	1/1	0.99	0.04	-3.69	33,33,33,33	0
2	CU	D	601	1/1	0.99	0.06	-3.76	19,19,19,19	0
2	CU	C	602	1/1	0.99	0.06	-4.01	21,21,21,21	0
2	CU	C	604	1/1	0.98	0.06	-4.26	30,30,30,30	0
2	CU	B	604	1/1	0.99	0.04	-4.61	26,26,26,26	0
2	CU	A	604	1/1	0.98	0.08	-5.39	27,27,27,27	0
2	CU	A	602	1/1	1.00	0.07	-6.72	11,11,11,11	0
2	CU	A	603	1/1	0.99	0.06	-8.22	14,14,14,14	0
6	NAG	B	770	14/15	0.96	0.13	-	17,27,34,34	0
6	NAG	A	720	14/15	0.97	0.11	-	15,20,29,44	0
6	NAG	A	730	14/15	0.92	0.17	-	13,31,41,56	0
6	NAG	C	730	14/15	0.92	0.17	-	19,29,44,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.