wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2023 – 05:59 PM EDT

PDB ID	:	1KYA
Title	:	ACTIVE LACCASE FROM TRAMETES VERSICOLOR COMPLEXED WITH 2,5-XYLIDINE
Authors	:	Bertrand, T.; Jolivalt, C.; Briozzo, P.; Caminade, E.; Joly, N.; Madzak, C.; Mougin, C.
Deposited on	:	2002-02-04
Resolution	:	2.40 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

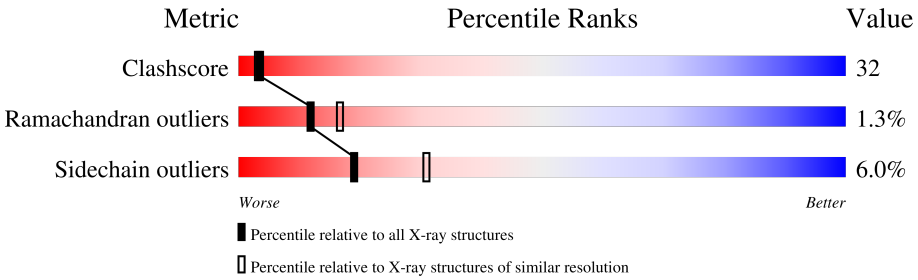
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	499	59% 36%
1	B	499	61% 34%
1	C	499	63% 33%
1	D	499	62% 34%

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	NAG	A	505	-	-	X	-
2	NAG	A	506	-	-	X	-
2	NAG	A	512	-	-	X	-
2	NAG	B	605	-	-	X	-
2	NAG	B	606	-	-	X	-
2	NAG	C	706	-	-	X	-
2	NAG	C	707	-	-	X	-
2	NAG	D	805	-	-	X	-
2	NAG	D	806	-	-	X	-
4	PYE	A	508	-	-	X	-
4	PYE	B	608	-	-	X	-
4	PYE	B	614	-	-	X	-
4	PYE	B	616	-	-	X	-
4	PYE	D	808	-	-	X	-
4	PYE	D	810	-	-	X	-
5	XYD	B	612	-	X	-	-
5	XYD	C	712	-	X	-	-

2 Entry composition (i)

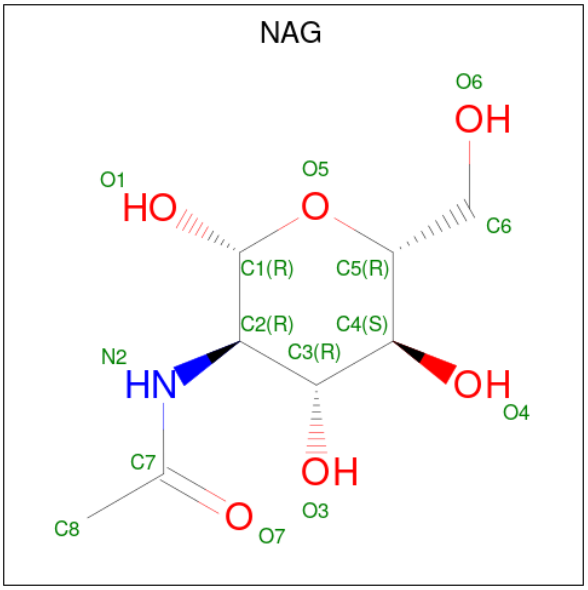
There are 6 unique types of molecules in this entry. The entry contains 16286 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	499	Total	C	N	O	S	0	0	0
			3753	2389	633	722	9			
1	B	499	Total	C	N	O	S	0	0	0
			3753	2389	633	722	9			
1	C	499	Total	C	N	O	S	0	0	0
			3753	2389	633	722	9			
1	D	499	Total	C	N	O	S	0	0	0
			3753	2389	633	722	9			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

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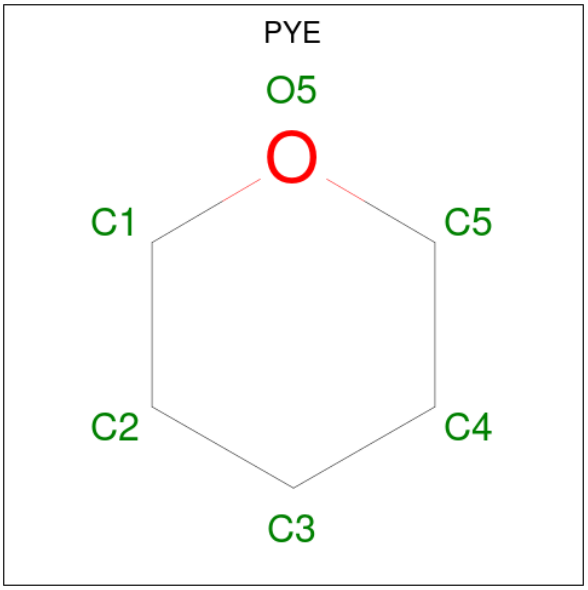
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Cu 4 4	0	0
3	B	4	Total Cu 4 4	0	0
3	C	4	Total Cu 4 4	0	0
3	D	4	Total Cu 4 4	0	0

- Molecule 4 is TETRAHYDROPYRAN (three-letter code: PYE) (formula: $C_5H_{10}O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 5 1	0	0

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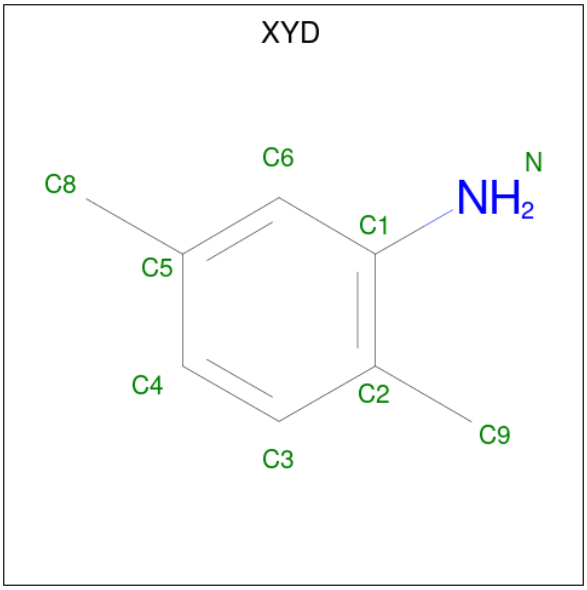
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 5 1	0	0
4	B	1	Total C O 6 5 1	0	0
4	B	1	Total C O 6 5 1	0	0
4	B	1	Total C O 6 5 1	0	0
4	B	1	Total C O 6 5 1	0	0
4	D	1	Total C O 6 5 1	0	0
4	D	1	Total C O 6 5 1	0	0
4	D	1	Total C O 6 5 1	0	0

- Molecule 5 is 2,5-DIMETHYLANILINE (three-letter code: XYD) (formula: $C_8H_{11}N$).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C N 9 8 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	184	Total O 184 184	0	0
6	B	209	Total O 209 209	0	0
6	C	199	Total O 199 199	0	0
6	D	198	Total O 198 198	0	0

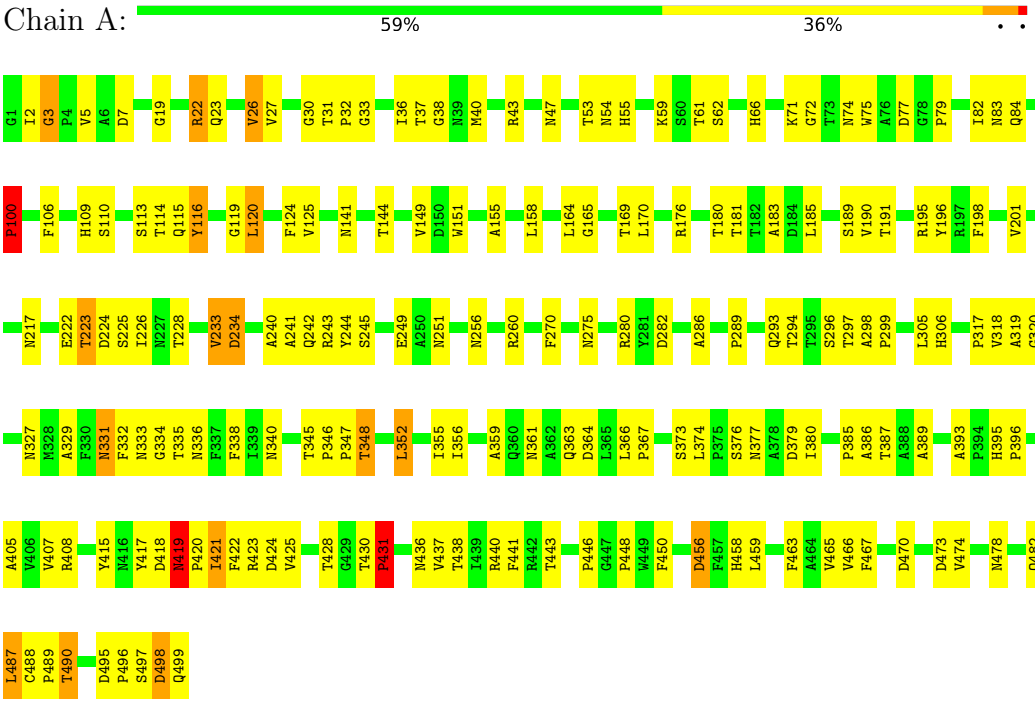
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

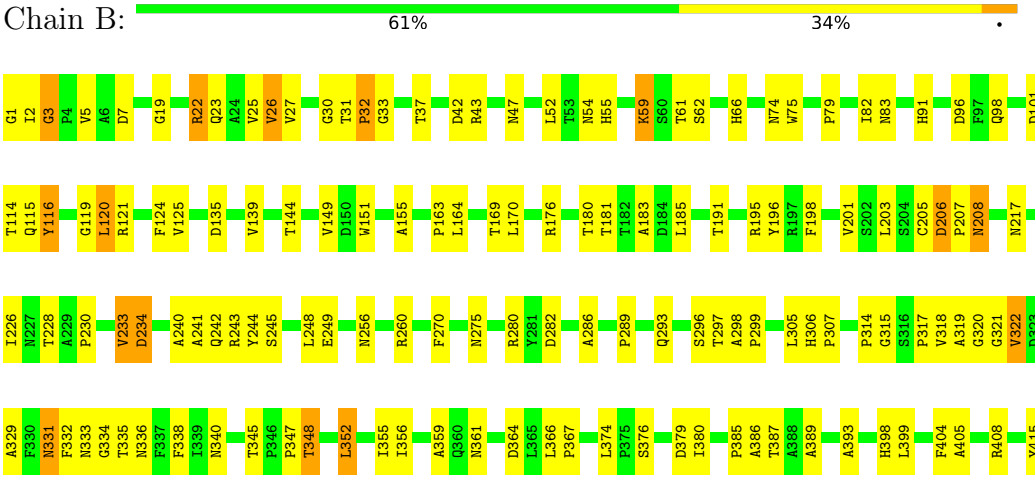
• Molecule 1: LACCASE

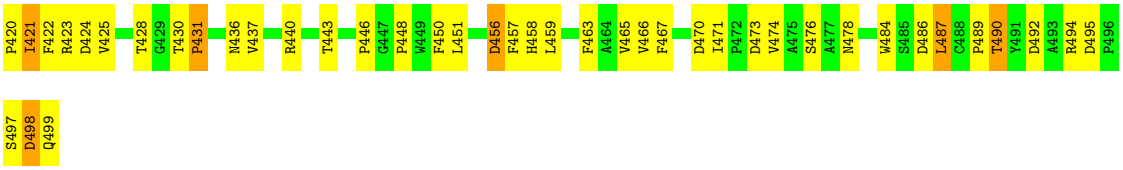
Chain A:



• Molecule 1: LACCASE

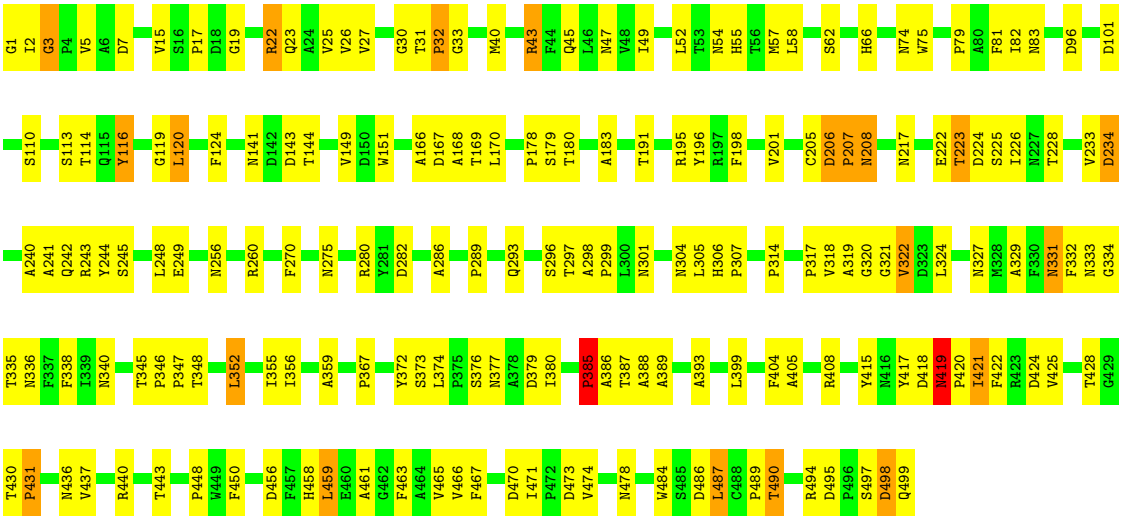
Chain B:





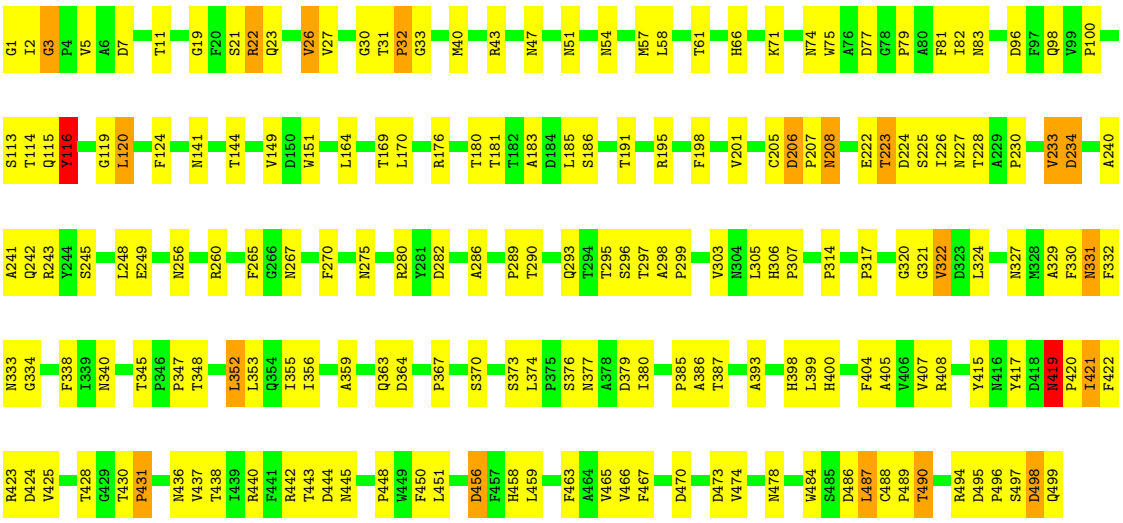
• Molecule 1: LACCASE

Chain C:



• Molecule 1: LACCASE

Chain D:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.72Å 110.52Å 123.20Å 90.00° 103.44° 90.00°	Depositor
Resolution (Å)	35.00 – 2.40	Depositor
% Data completeness (in resolution range)	93.5 (35.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.253 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16286	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PYE, XYD, NAG, CU

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	0.48	2/3867 (0.1%)	0.73	5/5320 (0.1%)
1	B	0.46	1/3867 (0.0%)	0.70	2/5320 (0.0%)
1	C	0.47	0/3867	0.70	4/5320 (0.1%)
1	D	0.47	0/3867	0.71	3/5320 (0.1%)
All	All	0.47	3/15468 (0.0%)	0.71	14/21280 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	431	PRO	N-CA	5.74	1.57	1.47
1	A	100	PRO	N-CA	5.54	1.56	1.47
1	B	431	PRO	N-CA	5.01	1.55	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	207	PRO	CA-N-CD	-8.80	99.18	111.50
1	A	100	PRO	CA-N-CD	-8.21	100.01	111.50
1	A	431	PRO	CA-N-CD	-7.40	101.14	111.50
1	A	100	PRO	N-CA-C	6.91	130.07	112.10
1	C	207	PRO	CA-N-CD	-6.53	102.36	111.50

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	3753	0	3541	252	0
1	B	3753	0	3541	226	0
1	C	3753	0	3539	222	0
1	D	3753	0	3541	211	0
2	A	98	0	91	32	0
2	B	98	0	91	26	0
2	C	98	0	91	21	0
2	D	84	0	78	20	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	12	0	20	4	0
4	B	24	0	40	14	0
4	D	18	0	30	10	0
5	A	9	0	11	4	0
5	B	9	0	11	3	0
5	C	9	0	11	2	0
5	D	9	0	11	3	0
6	A	184	0	0	78	3
6	B	209	0	0	63	1
6	C	199	0	0	63	1
6	D	198	0	0	46	0
All	All	16286	0	14647	964	3

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 32.

The worst 5 of 964 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:D:332:PHE:CZ	1:D:334:GLY:O	1.72	1.39
1:D:54:ASN:HD21	2:D:806:NAG:C1	1.44	1.30
1:B:366:LEU:HG	6:B:1525:HOH:O	1.23	1.27
1:C:436:ASN:HD21	2:C:707:NAG:C1	1.46	1.26
1:C:54:ASN:HD21	2:C:706:NAG:C1	1.48	1.26

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1560:HOH:O	6:A:1705:HOH:O[2_556]	1.63	0.57
6:A:1584:HOH:O	6:C:1103:HOH:O[2_646]	2.17	0.03
6:A:1491:HOH:O	6:B:1592:HOH:O[2_646]	2.19	0.01

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	497/499 (100%)	461 (93%)	30 (6%)	6 (1%)	13	19
1	B	497/499 (100%)	463 (93%)	27 (5%)	7 (1%)	11	15
1	C	497/499 (100%)	460 (93%)	30 (6%)	7 (1%)	11	15
1	D	497/499 (100%)	466 (94%)	25 (5%)	6 (1%)	13	19
All	All	1988/1996 (100%)	1850 (93%)	112 (6%)	26 (1%)	12	17

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	GLY
1	B	3	GLY
1	C	3	GLY
1	D	3	GLY
1	A	498	ASP

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	402/407 (99%)	375 (93%)	27 (7%)	16	26
1	B	402/407 (99%)	379 (94%)	23 (6%)	20	33
1	C	402/407 (99%)	379 (94%)	23 (6%)	20	33
1	D	402/407 (99%)	379 (94%)	23 (6%)	20	33
All	All	1608/1628 (99%)	1512 (94%)	96 (6%)	19	31

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	233	VAL
1	C	487	LEU
1	C	322	VAL
1	C	399	LEU
1	D	116	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	419	ASN
1	D	306	HIS
1	C	478	ASN
1	D	115	GLN
1	D	336	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 56 ligands modelled in this entry, 16 are monoatomic - leaving 40 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	C	705	-	14,14,15	0.74	0	17,19,21	0.80	1 (5%)
2	NAG	A	507	-	14,14,15	0.50	0	17,19,21	0.62	0
2	NAG	C	707	-	14,14,15	0.49	0	17,19,21	0.77	1 (5%)
2	NAG	A	511	-	14,14,15	0.48	0	17,19,21	0.73	1 (5%)
5	XYD	C	712	-	9,9,9	6.07	6 (66%)	12,12,12	3.03	3 (25%)
5	XYD	D	814	-	9,9,9	6.36	6 (66%)	12,12,12	2.67	2 (16%)
4	PYE	D	809	-	6,6,6	0.90	0	6,6,6	0.44	0
4	PYE	A	508	-	6,6,6	0.77	0	6,6,6	0.42	0
4	PYE	B	615	-	6,6,6	0.81	0	6,6,6	0.41	0
4	PYE	B	608	-	6,6,6	0.76	0	6,6,6	0.47	0
2	NAG	A	510	-	14,14,15	0.60	0	17,19,21	0.67	0
2	NAG	D	811	-	14,14,15	0.50	0	17,19,21	0.69	1 (5%)
2	NAG	D	806	-	14,14,15	0.71	0	17,19,21	0.78	0
2	NAG	B	610	-	14,14,15	0.55	0	17,19,21	0.65	1 (5%)
2	NAG	B	613	-	14,14,15	0.50	0	17,19,21	0.73	0
2	NAG	D	805	-	14,14,15	0.55	0	17,19,21	0.84	1 (5%)
2	NAG	A	512	-	14,14,15	0.41	0	17,19,21	0.72	0
2	NAG	A	505	-	14,14,15	0.47	0	17,19,21	0.83	0
2	NAG	A	513	-	14,14,15	0.62	0	17,19,21	0.88	1 (5%)
4	PYE	B	614	-	6,6,6	0.85	0	6,6,6	0.40	0
4	PYE	D	808	-	6,6,6	0.80	0	6,6,6	0.55	0
2	NAG	C	706	-	14,14,15	0.55	0	17,19,21	0.69	0
2	NAG	B	607	-	14,14,15	0.64	0	17,19,21	0.66	1 (5%)
2	NAG	B	611	-	14,14,15	0.47	0	17,19,21	0.64	0
5	XYD	A	514	-	9,9,9	6.30	5 (55%)	12,12,12	2.75	3 (25%)
4	PYE	A	509	-	6,6,6	0.75	0	6,6,6	0.46	0
2	NAG	D	813	-	14,14,15	0.49	0	17,19,21	0.62	0
4	PYE	D	810	-	6,6,6	0.87	0	6,6,6	0.41	0
2	NAG	B	605	-	14,14,15	0.59	0	17,19,21	0.56	0
2	NAG	C	711	-	14,14,15	0.61	0	17,19,21	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	XYD	B	612	-	9,9,9	6.27	6 (66%)	12,12,12	2.74	3 (25%)
2	NAG	C	709	-	14,14,15	0.57	0	17,19,21	0.53	0
2	NAG	C	708	-	14,14,15	0.45	0	17,19,21	0.70	1 (5%)
2	NAG	B	606	-	14,14,15	0.80	0	17,19,21	1.65	2 (11%)
4	PYE	B	616	-	6,6,6	0.78	0	6,6,6	0.43	0
2	NAG	A	506	-	14,14,15	0.62	0	17,19,21	0.82	0
2	NAG	D	807	-	14,14,15	0.54	0	17,19,21	0.72	1 (5%)
2	NAG	D	812	-	14,14,15	0.57	0	17,19,21	0.62	0
2	NAG	C	710	-	14,14,15	0.48	0	17,19,21	0.73	1 (5%)
2	NAG	B	609	-	14,14,15	0.54	0	17,19,21	0.98	1 (5%)

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	NAG	C	705	-	-	5/6/23/26	0/1/1/1
2	NAG	A	507	-	-	3/6/23/26	0/1/1/1
2	NAG	C	707	-	-	2/6/23/26	0/1/1/1
2	NAG	A	511	-	-	4/6/23/26	0/1/1/1
5	XYD	C	712	-	-	-	0/1/1/1
5	XYD	D	814	-	-	-	0/1/1/1
4	PYE	D	809	-	-	-	0/1/1/1
4	PYE	A	508	-	-	-	0/1/1/1
4	PYE	B	615	-	-	-	0/1/1/1
4	PYE	B	608	-	-	-	0/1/1/1
2	NAG	A	510	-	-	2/6/23/26	0/1/1/1
2	NAG	D	811	-	-	2/6/23/26	0/1/1/1
2	NAG	D	806	-	-	0/6/23/26	0/1/1/1
2	NAG	B	610	-	-	4/6/23/26	0/1/1/1
2	NAG	B	613	-	-	3/6/23/26	0/1/1/1
2	NAG	D	805	-	-	2/6/23/26	0/1/1/1
2	NAG	A	512	-	-	4/6/23/26	0/1/1/1
2	NAG	A	505	-	-	4/6/23/26	0/1/1/1
2	NAG	A	513	-	-	2/6/23/26	0/1/1/1
4	PYE	B	614	-	-	-	0/1/1/1
4	PYE	D	808	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	706	-	-	2/6/23/26	0/1/1/1
2	NAG	B	607	-	-	2/6/23/26	0/1/1/1
2	NAG	B	611	-	-	4/6/23/26	0/1/1/1
5	XYD	A	514	-	-	-	0/1/1/1
4	PYE	A	509	-	-	-	0/1/1/1
2	NAG	D	813	-	-	4/6/23/26	0/1/1/1
4	PYE	D	810	-	-	-	0/1/1/1
2	NAG	B	605	-	-	3/6/23/26	0/1/1/1
2	NAG	C	711	-	-	6/6/23/26	0/1/1/1
5	XYD	B	612	-	-	-	0/1/1/1
2	NAG	C	709	-	-	4/6/23/26	0/1/1/1
2	NAG	C	708	-	-	4/6/23/26	0/1/1/1
2	NAG	B	606	-	-	2/6/23/26	0/1/1/1
4	PYE	B	616	-	-	-	0/1/1/1
2	NAG	A	506	-	-	0/6/23/26	0/1/1/1
2	NAG	D	807	-	-	1/6/23/26	0/1/1/1
2	NAG	D	812	-	-	5/6/23/26	0/1/1/1
2	NAG	C	710	-	-	3/6/23/26	0/1/1/1
2	NAG	B	609	-	-	2/6/23/26	0/1/1/1

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	814	XYD	C6-C1	10.03	1.54	1.40
5	B	612	XYD	C6-C1	9.88	1.54	1.40
5	C	712	XYD	C6-C1	9.73	1.54	1.40
5	A	514	XYD	C6-C5	9.66	1.55	1.39
5	A	514	XYD	C6-C1	9.53	1.54	1.40

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	712	XYD	C1-C6-C5	-9.41	117.99	122.18
5	A	514	XYD	C1-C6-C5	-8.51	118.39	122.18
5	B	612	XYD	C1-C6-C5	-8.40	118.44	122.18
5	D	814	XYD	C1-C6-C5	-8.15	118.55	122.18
2	B	606	NAG	C3-C4-C5	4.17	117.68	110.24

There are no chirality outliers.

5 of 79 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	507	NAG	C8-C7-N2-C2
2	A	507	NAG	O7-C7-N2-C2
2	A	510	NAG	C8-C7-N2-C2
2	A	510	NAG	O7-C7-N2-C2
2	A	511	NAG	C8-C7-N2-C2

There are no ring outliers.

38 monomers are involved in 127 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	705	NAG	4	0
2	A	507	NAG	2	0
2	C	707	NAG	8	0
5	C	712	XYD	2	0
5	D	814	XYD	3	0
4	D	809	PYE	2	0
4	A	508	PYE	4	0
4	B	615	PYE	2	0
4	B	608	PYE	9	0
2	A	510	NAG	4	0
2	D	811	NAG	3	0
2	D	806	NAG	7	0
2	B	610	NAG	4	0
2	B	613	NAG	2	0
2	D	805	NAG	8	0
2	A	512	NAG	11	0
2	A	505	NAG	9	0
2	A	513	NAG	2	0
4	B	614	PYE	4	0
4	D	808	PYE	10	0
2	C	706	NAG	7	0
2	B	607	NAG	4	0
2	B	611	NAG	3	0
5	A	514	XYD	4	0
4	A	509	PYE	2	0
4	D	810	PYE	4	0
2	B	605	NAG	10	0
2	C	711	NAG	3	0
5	B	612	XYD	3	0
2	C	709	NAG	1	0
2	C	708	NAG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	606	NAG	7	0
4	B	616	PYE	5	0
2	A	506	NAG	9	0
2	D	807	NAG	3	0
2	D	812	NAG	5	0
2	C	710	NAG	1	0
2	B	609	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.