



Full wwPDB X-ray Structure Validation Report i

Sep 26, 2014 – 12:07 PM EDT

PDB ID : 4CVU
Title : Structure of Fungal beta-mannosidase from Glycoside Hydrolase Family 2 of *Trichoderma harzianum*
Authors : Muniz, J.R.C.; Aparicio, R.; Santos, J.C.; Nascimento, A.S.; Golubev, A.M.; Polikarpov, I.
Deposited on : 2014-03-31
Resolution : 1.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

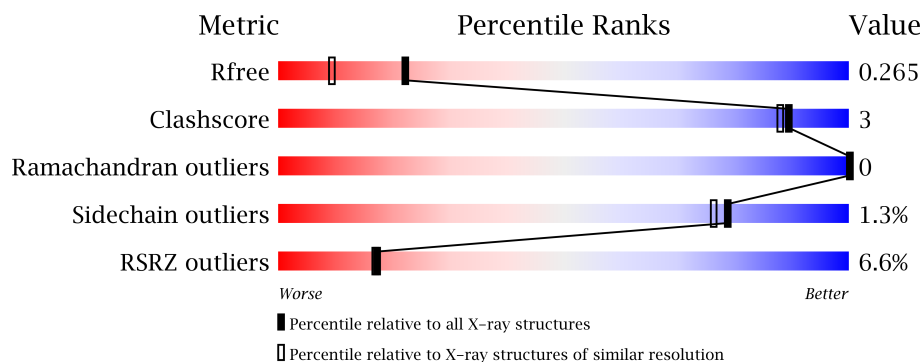
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : trunk23956
Percentile statistics : 23426
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk23956

1 Overall quality at a glance

The reported resolution of this entry is 1.90 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}	77520	4208 (1.90-1.90)
Clashscore	88313	4838 (1.90-1.90)
Ramachandran outliers	86584	4785 (1.90-1.90)
C α geometry	86677	4778 (1.90-1.90)
Sidechain outliers	86556	4786 (1.90-1.90)
RSRZ outliers	77580	4210 (1.90-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	942	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	NAG	A	1974	-	X
8	CD	A	1991	-	X
8	CD	A	1993	-	X
9	NA	A	1995	-	X
9	NA	A	1996	-	X
9	NA	A	1997	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
9	NA	A	2004	-	X

2 Entry composition i

There are 14 unique types of molecules in this entry. The entry contains 8456 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

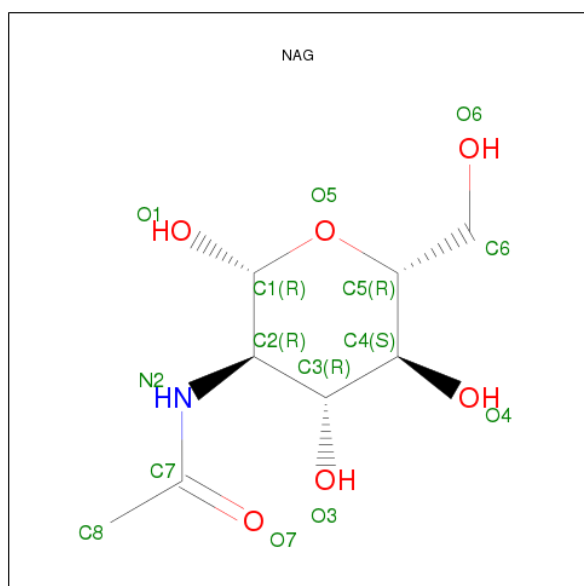
- Molecule 1 is a protein called BETA-MANNOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	913	7241	4645	1208	1371	17	0	6	0

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	8	Total	C	N	O	0	0
			94	52	2	40		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	11	Total	C	N	O	0	0
			127	70	2	55		

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

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

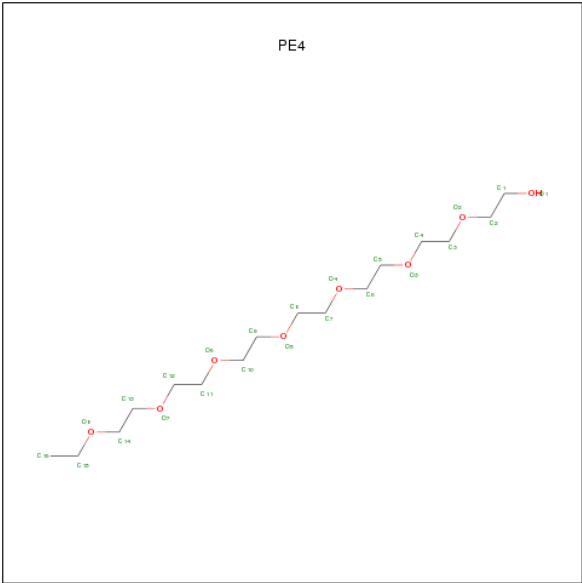
- Molecule 8 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	17	Total	Cd	0	0
			17	17		

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

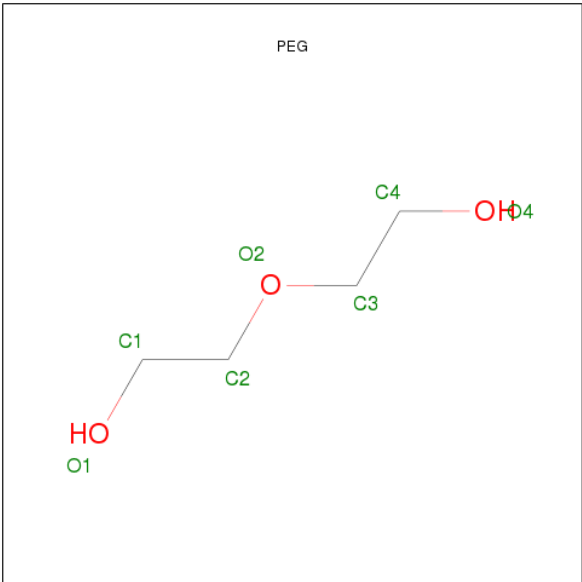
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	6	Total	Na		0	0
			6	6			

- Molecule 10 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: C₁₆H₃₄O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			12	8	4		

- Molecule 11 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 12 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 13 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 14 is water.

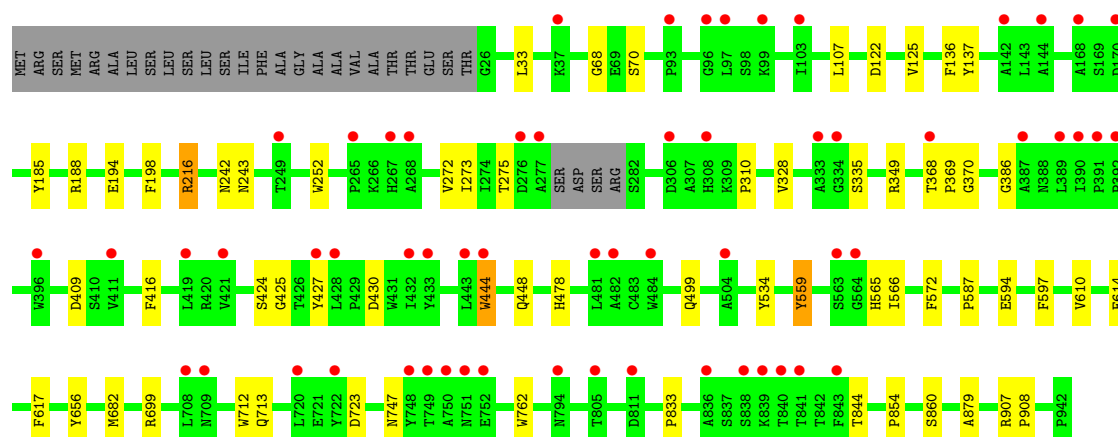
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	741	Total	O	0	0
			741	741		

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: BETA-MANNOSIDASE

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	166.46Å 166.46Å 121.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	117.70 – 1.90 48.30 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (117.70-1.90) 98.8 (48.30-1.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.234 , 0.263 0.239 , 0.265	Depositor DCC
R_{free} test set	6636 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 131627 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8456	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: BMA, NAG, CL, PE4, NA, CA, CD, PEG, 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	0.67	0/7479	0.72	4/10243 (0.0%)

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
1	A	0	1
7	A	1	0
All	All	1	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	723	ASP	CB-CG-OD1	6.79	124.41	118.30
1	A	409	ASP	CB-CG-OD1	6.43	124.09	118.30
1	A	723	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	A	188	ARG	NE-CZ-NH2	5.04	122.82	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	1977	NAG	C3

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	424	SER	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7241	0	6832	39	0
2	A	39	0	34	1	0
3	A	70	0	65	0	0
4	A	94	0	79	1	0
5	A	72	0	61	0	0
6	A	127	0	105	0	0
7	A	28	0	23	0	0
8	A	17	0	0	0	0
9	A	6	0	0	0	0
10	A	12	0	14	0	0
11	A	7	0	10	0	0
12	A	1	0	0	0	0
13	A	1	0	0	1	0
14	A	741	0	0	7	0
All	All	8456	0	7223	40	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (40) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:1948:NAG:H81	4:A:1953:MAN:O6	1.81	0.80
1:A:194:GLU:HG3	1:A:425:GLY:HA2	1.67	0.75
1:A:597:PHE:HB2	1:A:682:MET:CE	2.26	0.66
1:A:565:HIS:NE2	13:A:2003:CL:CL	2.58	0.65
1:A:597:PHE:HB2	1:A:682:MET:HE1	1.80	0.64
1:A:844:THR:O	14:A:3586:HOH:O	2.16	0.62
1:A:879:ALA:O	1:A:908:PRO:HA	2.03	0.58
1:A:656:TYR:CE1	1:A:854:PRO:HG2	2.41	0.55
1:A:444:TRP:CD1	1:A:444:TRP:C	2.80	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:860:SER:OG	14:A:3647:HOH:O	2.18	0.53
1:A:272:VAL:HG12	1:A:328:VAL:HG22	1.91	0.52
1:A:617:PHE:CD1	2:A:1943:NAG:H82	2.45	0.51
1:A:107:LEU:O	1:A:136:PHE:HA	2.11	0.51
1:A:243:ASN:HD21	1:A:534:TYR:H	1.57	0.51
1:A:610[A]:VAL:CG1	1:A:614:GLU:HB2	2.42	0.50
1:A:572:PHE:CD1	1:A:587:PRO:HD3	2.46	0.49
1:A:597:PHE:HB2	1:A:682:MET:HE2	1.96	0.48
1:A:194:GLU:HG3	1:A:425:GLY:CA	2.42	0.47
1:A:594:GLU:CD	14:A:3402:HOH:O	2.53	0.47
1:A:335:SER:CB	14:A:3290:HOH:O	2.63	0.47
1:A:185:TYR:HB2	1:A:198:PHE:HB3	1.98	0.46
1:A:747:ASN:ND2	14:A:3595:HOH:O	2.39	0.46
1:A:242:ASN:O	1:A:243:ASN:HB2	2.16	0.45
1:A:430:ASP:OD1	1:A:478:HIS:CE1	2.69	0.45
1:A:427:TYR:CE2	1:A:448:GLN:HG2	2.51	0.45
1:A:713:GLN:OE1	1:A:713:GLN:N	2.46	0.45
1:A:762:TRP:CE3	1:A:833:PRO:HB3	2.53	0.44
1:A:125[A]:VAL:HG12	1:A:137:TYR:HB3	1.99	0.44
1:A:860:SER:CB	14:A:3647:HOH:O	2.65	0.43
1:A:273:ILE:HG22	1:A:275[B]:THR:HG23	2.01	0.42
1:A:368:THR:HA	1:A:369:PRO:HD3	1.87	0.42
1:A:33:LEU:HG	1:A:216:ARG:HA	2.01	0.42
1:A:252:TRP:CD1	1:A:310:PRO:HG2	2.55	0.42
1:A:559:TYR:N	1:A:559:TYR:CD1	2.86	0.42
1:A:370:GLY:HA3	1:A:566:ILE:O	2.20	0.41
1:A:444:TRP:C	1:A:444:TRP:HD1	2.22	0.41
1:A:386:GLY:HA2	1:A:416:PHE:CD2	2.55	0.41
1:A:610[A]:VAL:HG13	1:A:614:GLU:HB2	2.02	0.41
1:A:68:GLY:HA3	14:A:3051:HOH:O	2.20	0.41
1:A:243:ASN:HD21	1:A:534:TYR:N	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	915/942 (97%)	891 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	777/811 (96%)	766 (99%)	11 (1%)	77	74

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	SER
1	A	122	ASP
1	A	216	ARG
1	A	349[A]	ARG
1	A	349[B]	ARG
1	A	444	TRP
1	A	499	GLN
1	A	559	TYR
1	A	699	ARG
1	A	712	TRP
1	A	907	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	A	243	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

30 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	A	1943	1,2	14,14,15	0.63	0	19,19,21	1.43	3 (15%)
2	NAG	A	1944	2	14,14,15	0.61	0	19,19,21	1.06	2 (10%)
2	BMA	A	1945	2	11,11,12	0.50	0	15,15,17	0.78	0
4	NAG	A	1947	1,4	14,14,15	0.79	1 (7%)	19,19,21	1.00	1 (5%)
4	NAG	A	1948	4	14,14,15	0.63	0	19,19,21	1.32	3 (15%)
4	BMA	A	1949	4	11,11,12	0.76	0	15,15,17	1.13	2 (13%)
4	MAN	A	1950	4	11,11,12	0.58	0	15,15,17	0.90	0
4	MAN	A	1951	4	11,11,12	0.51	0	15,15,17	1.07	1 (6%)
4	MAN	A	1952	4	11,11,12	0.59	0	15,15,17	2.21	2 (13%)
4	MAN	A	1953	4	11,11,12	0.73	0	15,15,17	1.52	3 (20%)
4	MAN	A	1954	4	11,11,12	0.65	0	15,15,17	0.93	1 (6%)
5	NAG	A	1955	1,5	14,14,15	0.49	0	19,19,21	1.28	3 (15%)
5	NAG	A	1956	5	14,14,15	0.71	0	19,19,21	1.27	2 (10%)
5	BMA	A	1957	5	11,11,12	0.58	0	15,15,17	1.14	1 (6%)
5	MAN	A	1958	5	11,11,12	0.60	0	15,15,17	1.31	1 (6%)
5	MAN	A	1959	5	11,11,12	0.58	0	15,15,17	1.04	1 (6%)
5	MAN	A	1960	5	11,11,12	0.96	0	15,15,17	5.62	3 (20%)
6	NAG	A	1961	1,6	14,14,15	0.64	0	19,19,21	1.30	2 (10%)
6	NAG	A	1962	6	14,14,15	0.74	0	19,19,21	0.91	1 (5%)
6	BMA	A	1963	6	11,11,12	0.51	0	15,15,17	0.89	1 (6%)
6	MAN	A	1964	6	11,11,12	0.59	0	15,15,17	1.12	1 (6%)
6	MAN	A	1965	6	11,11,12	0.99	0	15,15,17	1.14	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	A	1966	6	11,11,12	0.59	0	15,15,17	1.16	2 (13%)
6	MAN	A	1967	6	11,11,12	1.36	1 (9%)	15,15,17	3.38	3 (20%)
6	MAN	A	1968	6	11,11,12	0.72	0	15,15,17	0.88	0
6	MAN	A	1969	6	11,11,12	0.62	0	15,15,17	0.77	1 (6%)
6	MAN	A	1970	6	11,11,12	0.71	0	15,15,17	1.53	4 (26%)
6	MAN	A	1971	6	11,11,12	0.69	0	15,15,17	1.38	1 (6%)
7	NAG	A	1976	1,7	14,14,15	0.91	1 (7%)	19,19,21	1.41	2 (10%)
7	NAG	A	1977	7	14,14,15	25.63	1 (7%)	19,19,21	8.90	9 (47%)

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	A	1943	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1944	2	-	0/6/23/26	0/1/1/1
2	BMA	A	1945	2	-	0/2/19/22	0/1/1/1
4	NAG	A	1947	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1948	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1949	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1950	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1951	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1952	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1953	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1954	4	-	0/2/19/22	0/1/1/1
5	NAG	A	1955	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1956	5	-	0/6/23/26	0/1/1/1
5	BMA	A	1957	5	-	0/2/19/22	0/1/1/1
5	MAN	A	1958	5	-	0/2/19/22	0/1/1/1
5	MAN	A	1959	5	-	0/2/19/22	0/1/1/1
5	MAN	A	1960	5	-	0/2/18/22	0/1/1/1
6	NAG	A	1961	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1962	6	-	0/6/23/26	0/1/1/1
6	BMA	A	1963	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1964	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1965	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1966	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1967	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1968	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1969	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	A	1970	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1971	6	-	0/2/19/22	0/1/1/1
7	NAG	A	1976	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1977	7	1/1/5/7	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1977	NAG	O3-C3	95.86	3.75	1.43
6	A	1967	MAN	O3-C3	-3.91	1.33	1.43
4	A	1947	NAG	C1-C2	2.13	1.55	1.52
7	A	1976	NAG	O5-C1	-2.04	1.40	1.43

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1977	NAG	O3-C3-C2	-37.04	21.26	109.61
5	A	1960	MAN	O5-C1-C2	20.03	126.31	110.72
6	A	1967	MAN	O3-C3-C2	12.28	132.35	110.00
7	A	1977	NAG	O3-C3-C4	-6.86	95.03	110.36
5	A	1960	MAN	C1-C2-C3	-6.23	100.55	111.23
4	A	1952	MAN	C1-O5-C5	6.23	120.14	112.13
5	A	1960	MAN	C3-C4-C5	5.16	115.22	109.92
7	A	1977	NAG	C8-C7-N2	4.61	124.83	116.12
4	A	1952	MAN	O5-C5-C4	4.26	119.30	110.75
7	A	1977	NAG	O5-C1-C2	-4.16	107.49	111.68
7	A	1977	NAG	C2-N2-C7	4.15	128.75	123.42
6	A	1961	NAG	O5-C1-C2	-3.90	107.75	111.68
2	A	1943	NAG	O5-C1-C2	-3.48	108.17	111.68
7	A	1976	NAG	C1-O5-C5	3.46	116.58	112.13
7	A	1976	NAG	O5-C1-C2	-3.41	108.25	111.68
4	A	1953	MAN	C1-C2-C3	3.41	113.89	109.65
5	A	1955	NAG	O5-C1-C2	-3.18	108.48	111.68
6	A	1971	MAN	C1-O5-C5	3.13	116.15	112.13
4	A	1954	MAN	C1-O5-C5	3.13	116.15	112.13
4	A	1948	NAG	C2-N2-C7	3.12	127.42	123.42
4	A	1951	MAN	C1-O5-C5	3.07	116.08	112.13
5	A	1958	MAN	O2-C2-C3	-2.97	104.49	110.24
6	A	1970	MAN	O5-C1-C2	2.97	115.49	110.84
6	A	1961	NAG	C1-O5-C5	2.80	115.73	112.13
6	A	1966	MAN	C2-C3-C4	-2.74	106.30	110.99
4	A	1949	BMA	O3-C3-C4	-2.69	104.36	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1970	MAN	C3-C4-C5	2.67	114.97	110.17
2	A	1943	NAG	C1-O5-C5	2.67	115.56	112.13
5	A	1957	BMA	O4-C4-C3	-2.62	104.49	110.36
6	A	1970	MAN	C1-C2-C3	-2.58	106.44	109.65
6	A	1965	MAN	C1-O5-C5	2.56	115.42	112.13
5	A	1955	NAG	C1-O5-C5	2.47	115.30	112.13
5	A	1956	NAG	C3-C4-C5	-2.45	105.78	110.17
6	A	1969	MAN	C1-O5-C5	2.40	115.22	112.13
5	A	1955	NAG	C1-C2-C3	2.39	112.93	109.15
2	A	1943	NAG	C1-C2-C3	2.37	112.89	109.15
7	A	1977	NAG	C3-C4-C5	2.35	114.39	110.17
7	A	1977	NAG	O7-C7-C8	-2.35	117.53	122.04
2	A	1944	NAG	C1-O5-C5	2.29	115.07	112.13
4	A	1953	MAN	O2-C2-C1	-2.26	104.41	109.09
4	A	1948	NAG	C8-C7-N2	2.25	120.38	116.12
6	A	1967	MAN	C1-O5-C5	2.21	114.98	112.13
6	A	1970	MAN	O4-C4-C3	-2.21	105.42	110.36
5	A	1956	NAG	O5-C1-C2	-2.19	109.48	111.68
2	A	1944	NAG	C1-C2-C3	2.15	112.55	109.15
5	A	1959	MAN	O5-C5-C6	2.15	110.67	106.97
6	A	1962	NAG	O7-C7-C8	-2.14	117.94	122.04
4	A	1948	NAG	O5-C1-C2	-2.11	109.55	111.68
7	A	1977	NAG	C3-C2-N2	2.11	115.75	110.50
6	A	1966	MAN	C1-O5-C5	2.10	114.83	112.13
7	A	1977	NAG	O7-C7-N2	-2.09	117.64	121.90
4	A	1947	NAG	C2-N2-C7	-2.09	120.74	123.42
4	A	1949	BMA	O4-C4-C3	-2.08	105.70	110.36
6	A	1964	MAN	O4-C4-C5	2.06	114.70	109.25
6	A	1963	BMA	O6-C6-C5	-2.04	104.25	111.37
4	A	1953	MAN	C1-O5-C5	2.04	114.75	112.13
6	A	1967	MAN	O3-C3-C4	-2.03	105.82	110.36
6	A	1965	MAN	C6-C5-C4	-2.00	108.15	113.04

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	1977	NAG	C3

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry

Of 32 ligands modelled in this entry, 25 are monoatomic - leaving 7 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	NAG	A	1946	1	14,14,15	0.89	0	19,19,21	1.53	2 (10%)
3	NAG	A	1972	1	14,14,15	0.46	0	19,19,21	1.23	1 (5%)
3	NAG	A	1973	1	14,14,15	0.41	0	19,19,21	1.79	4 (21%)
3	NAG	A	1974	1	14,14,15	0.52	0	19,19,21	1.45	3 (15%)
3	NAG	A	1975	1	14,14,15	0.50	0	19,19,21	1.12	2 (10%)
10	PE4	A	2000	-	11,11,23	0.55	0	10,10,22	0.44	0
11	PEG	A	2001	-	6,6,6	0.53	0	5,5,5	0.22	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
3	NAG	A	1946	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1972	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1973	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1974	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1975	1	-	0/6/23/26	0/1/1/1
10	PE4	A	2000	-	-	0/9/9/21	0/0/0/0
11	PEG	A	2001	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1946	NAG	C1-O5-C5	4.97	118.51	112.13
3	A	1973	NAG	O5-C1-C2	-4.31	107.34	111.68
3	A	1972	NAG	C1-O5-C5	3.75	116.95	112.13
3	A	1974	NAG	C1-C2-C3	3.54	114.74	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1973	NAG	C1-C2-C3	3.42	114.56	109.15
3	A	1973	NAG	C1-O5-C5	3.01	116.00	112.13
3	A	1974	NAG	O5-C1-C2	-3.01	108.65	111.68
3	A	1946	NAG	C1-C2-C3	2.76	113.52	109.15
3	A	1974	NAG	C1-O5-C5	2.60	115.47	112.13
3	A	1973	NAG	O5-C5-C6	2.43	111.16	106.97
3	A	1975	NAG	O5-C1-C2	-2.10	109.57	111.68
3	A	1975	NAG	C4-C3-C2	-2.08	108.20	111.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	913/942 (96%)	0.33	60 (6%) 17 17	28, 45, 69, 105	1 (0%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	334	GLY	6.4
1	A	749	THR	5.1
1	A	838	SER	5.1
1	A	267	HIS	4.0
1	A	839	LYS	4.0
1	A	751	ASN	4.0
1	A	389	LEU	3.6
1	A	421	VAL	3.6
1	A	443	LEU	3.5
1	A	563	SER	3.5
1	A	419	LEU	3.5
1	A	306	ASP	3.2
1	A	843	PHE	3.1
1	A	708	LEU	3.1
1	A	268	ALA	3.1
1	A	722	TYR	3.0
1	A	96	GLY	3.0
1	A	392	PRO	2.9
1	A	840	THR	2.9
1	A	333	ALA	2.9
1	A	277	ALA	2.9
1	A	504	ALA	2.8
1	A	750	ALA	2.8
1	A	391	PRO	2.8
1	A	390	ILE	2.7
1	A	428	LEU	2.7
1	A	265	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	97	LEU	2.6
1	A	481	LEU	2.6
1	A	564	GLY	2.5
1	A	168	ALA	2.5
1	A	276	ASP	2.5
1	A	752	GLU	2.5
1	A	37	LYS	2.5
1	A	805	THR	2.5
1	A	482	ALA	2.5
1	A	170	ASP	2.4
1	A	432	ILE	2.4
1	A	142	ALA	2.4
1	A	841	THR	2.4
1	A	444	TRP	2.3
1	A	387	ALA	2.3
1	A	308	HIS	2.2
1	A	836	ALA	2.2
1	A	103	ILE	2.1
1	A	396	TRP	2.1
1	A	748	TYR	2.1
1	A	709	ASN	2.1
1	A	368	THR	2.1
1	A	484	TRP	2.1
1	A	794	ASN	2.1
1	A	427	TYR	2.1
1	A	411	VAL	2.1
1	A	720	LEU	2.1
1	A	249	THR	2.1
1	A	93	PRO	2.0
1	A	811	ASP	2.0
1	A	144	ALA	2.0
1	A	433	TYR	2.0
1	A	99	LYS	2.0

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

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

6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	BMA	A	1949	11/12	0.21	13.12	50,55,57,59	0
7	NAG	A	1977	14/15	0.26	11.14	67,73,78,80	0
4	NAG	A	1948	14/15	0.20	8.05	44,48,53,54	0
4	MAN	A	1953	11/12	0.24	6.80	51,60,62,64	0
2	NAG	A	1944	14/15	0.18	6.64	46,50,51,52	0
4	MAN	A	1954	11/12	0.30	6.51	52,60,62,64	0
6	MAN	A	1971	11/12	0.15	4.00	51,53,54,56	0
4	MAN	A	1950	11/12	0.20	3.78	57,60,64,64	0
5	BMA	A	1957	11/12	0.13	3.01	48,51,55,58	0
6	MAN	A	1966	11/12	0.20	2.90	52,57,61,65	0
2	NAG	A	1943	14/15	0.12	2.80	35,38,42,45	0
4	NAG	A	1947	14/15	0.18	2.46	40,43,47,49	0
6	MAN	A	1965	11/12	0.16	2.37	45,48,53,57	0
5	NAG	A	1956	14/15	0.13	2.02	44,48,50,58	0
5	MAN	A	1958	11/12	0.11	1.99	43,46,47,48	0
7	NAG	A	1976	14/15	0.15	0.76	46,51,55,57	0
6	BMA	A	1963	11/12	0.11	0.33	43,45,50,50	0
5	NAG	A	1955	14/15	0.12	0.27	44,46,47,47	0
4	MAN	A	1951	11/12	0.13	0.20	57,61,64,69	0
5	MAN	A	1959	11/12	0.10	-0.10	43,47,53,56	0
6	MAN	A	1970	11/12	0.14	-0.16	48,55,62,63	0
6	NAG	A	1962	14/15	0.11	-0.39	41,44,47,48	0
6	MAN	A	1968	11/12	0.11	-0.46	46,50,52,53	0
6	MAN	A	1964	11/12	0.10	-0.92	43,44,47,48	0
6	MAN	A	1969	11/12	0.11	-1.18	49,51,52,52	0
6	NAG	A	1961	14/15	0.09	-1.71	42,45,51,51	0
2	BMA	A	1945	11/12	0.30	-	54,57,59,62	0
5	MAN	A	1960	11/12	0.18	-	65,66,68,70	0
6	MAN	A	1967	11/12	0.13	-	47,51,53,53	0
4	MAN	A	1952	11/12	0.40	-	63,65,67,68	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	RSR	LLDF	B-factors(Å ²)	Q<0.9
9	NA	A	1995	1/1	0.28	18.05	54,54,54,54	0
3	NAG	A	1974	14/15	0.29	9.00	54,59,68,70	0
9	NA	A	1997	1/1	0.24	7.01	30,30,30,30	0
8	CD	A	1991	1/1	0.20	6.16	125,125,125,125	1
9	NA	A	2004	1/1	0.32	5.93	37,37,37,37	0
9	NA	A	1996	1/1	0.26	3.58	48,48,48,48	0
8	CD	A	1993	1/1	0.38	2.17	44,44,44,44	0
3	NAG	A	1972	14/15	0.12	1.90	54,59,64,67	0
3	NAG	A	1973	14/15	0.27	1.58	56,60,63,68	0
10	PE4	A	2000	12/24	0.15	1.25	57,61,66,66	0
3	NAG	A	1975	14/15	0.13	0.97	40,43,46,47	0
11	PEG	A	2001	7/7	0.15	0.82	58,60,62,64	0
3	NAG	A	1946	14/15	0.10	0.02	39,44,48,48	0
13	CL	A	2003	1/1	0.15	-0.87	49,49,49,49	0
9	NA	A	1999	1/1	0.13	-0.93	33,33,33,33	0
8	CD	A	1979	1/1	0.07	-1.23	43,43,43,43	0
12	CA	A	2002	1/1	0.08	-1.35	54,54,54,54	0
8	CD	A	1978	1/1	0.08	-1.37	39,39,39,39	0
8	CD	A	1992	1/1	0.17	-1.60	87,87,87,87	1
9	NA	A	1998	1/1	0.14	-1.75	40,40,40,40	0
8	CD	A	1983	1/1	0.08	-1.76	52,52,52,52	0
8	CD	A	1985	1/1	0.07	-1.94	51,51,51,51	0
8	CD	A	1984	1/1	0.06	-2.19	76,76,76,76	0
8	CD	A	1990	1/1	0.08	-2.42	77,77,77,77	0
8	CD	A	1982	1/1	0.05	-2.56	72,72,72,72	0
8	CD	A	1981	1/1	0.05	-2.59	50,50,50,50	0
8	CD	A	1986	1/1	0.04	-3.07	59,59,59,59	0
8	CD	A	1980	1/1	0.08	-4.01	58,58,58,58	0
8	CD	A	1989	1/1	0.04	-6.31	80,80,80,80	0
8	CD	A	1987	1/1	0.08	-9.33	81,81,81,81	0
8	CD	A	1988	1/1	0.05	-	74,74,74,74	0
8	CD	A	1994	1/1	0.57	-	44,44,44,44	0

6.5 Other polymers ⓘ

There are no such residues in this entry.