



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 02:42 am GMT

PDB ID : 4UOJ
Title : Structure of Fungal beta-mannosidase (GH2) from Trichoderma hazianum
Authors : Muniz, J.R.C.; Aparicio, R.; Santos, J.C.; Nascimento, A.S.; Golubev, A.M.; Polikarpov, I.
Deposited on : 2014-06-04
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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

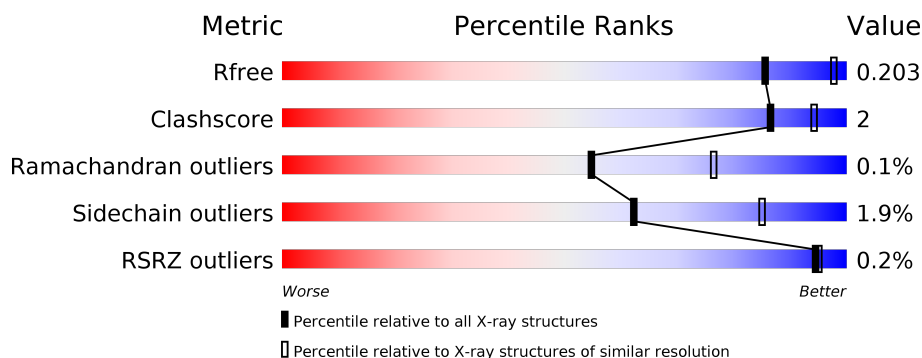
1 Overall quality at a glance

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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (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	942	
1	B	942	

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
11	PE4	A	1998	-	-	-	X
11	PE4	B	1995	-	-	-	X
12	MAN	B	1951	-	-	-	X
4	NAG	A	1979	-	-	-	X
6	MAN	A	1965	X	-	-	-
7	MAN	A	1975	-	-	-	X
9	NA	A	1996	-	-	-	X
9	NA	B	1992	-	-	-	X

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 16996 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 BETA-MANNOSIDASE GH2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	917	Total	C	N	O	S	0	2	0
			7259	4654	1213	1376	16			
1	B	917	Total	C	N	O	S	0	1	0
			7234	4634	1210	1374	16			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	6	Total	C	N	O	0	0
			72	40	2	30		
2	B	6	Total	C	N	O	0	0
			71	40	2	29		

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

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

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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	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	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		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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

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

- 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		
6	B	11	Total	C	N	O	0	0
			127	70	2	55		

- Molecule 7 is a polymer of unknown type called SUGAR (8-MER).

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	12	Total	Cd	0	0
			12	12		
8	A	16	Total	Cd	0	0
			16	16		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Na	0	0
			1	1		
9	A	2	Total	Na	0	0
			2	2		

- Molecule 10 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



- Molecule 11 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: C₁₆H₃₄O₈).



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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 12 is a polymer of unknown type called SUGAR (9-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	9	Total	C	N	O	0	0
			105	58	2	45		

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

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

- Molecule 14 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	B	1	Total	Ca	0	0
			1	1		

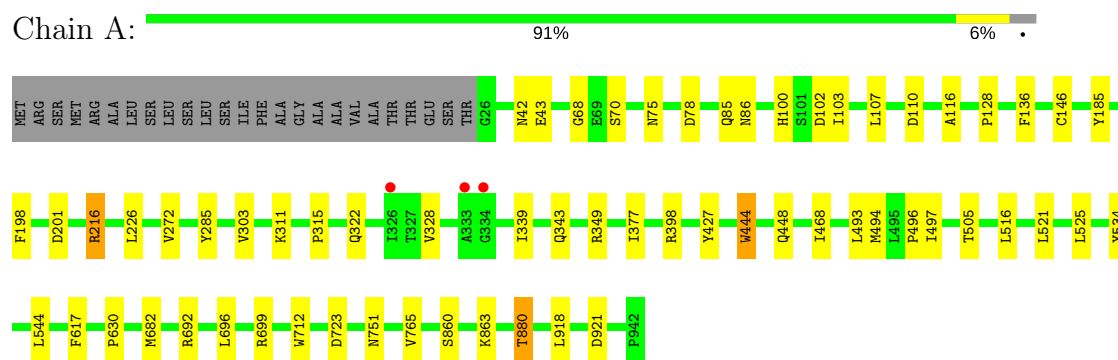
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	751	Total	O	0	0
			751	751		
15	B	749	Total	O	0	0
			749	749		

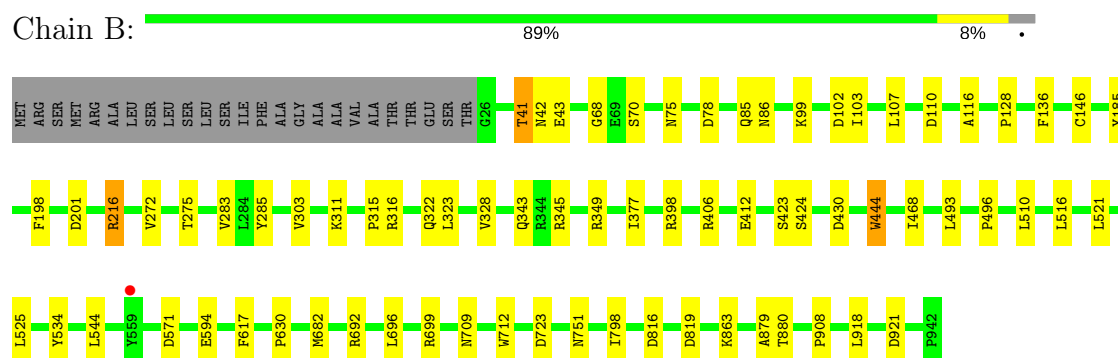
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 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 GH2



• Molecule 1: BETA-MANNOSIDASE GH2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	165.16Å 165.63Å 123.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	117.23 – 2.50 98.94 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (117.23-2.50) 99.1 (98.94-2.50)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.179 , 0.201 0.180 , 0.203	Depositor DCC
R_{free} test set	5871 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.350 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16996	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, 1PE, CD, 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	0.58	0/7491	0.67	1/10260 (0.0%)
1	B	0.59	0/7459	0.67	1/10217 (0.0%)
All	All	0.59	0/14950	0.67	2/20477 (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
6	A	1	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	723	ASP	CB-CG-OD1	5.94	123.65	118.30
1	B	723	ASP	CB-CG-OD1	5.76	123.48	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	1965	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	7259	0	6837	29	0
1	B	7234	0	6809	39	0
2	A	72	0	61	0	0
2	B	71	0	59	2	0
3	A	39	0	34	2	0
3	B	39	0	34	1	0
4	A	70	0	65	0	0
4	B	70	0	65	0	0
5	A	56	0	50	1	0
5	B	56	0	50	2	0
6	A	127	0	105	0	0
6	B	127	0	106	0	0
7	A	94	0	79	0	0
8	A	16	0	0	0	0
8	B	12	0	0	0	0
9	A	2	0	0	0	0
9	B	1	0	0	0	0
10	A	9	0	10	0	0
10	B	9	0	10	0	0
11	A	10	0	13	2	0
11	B	16	0	21	2	0
12	B	105	0	88	0	0
13	B	1	0	0	0	0
14	B	1	0	0	0	0
15	A	751	0	0	4	0
15	B	749	0	0	5	0
All	All	16996	0	14496	73	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 2.

The worst 5 of 73 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)
15:A:2741:HOH:O	1:B:68:GLY:HA3	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:LEU:HD13	1:B:345:ARG:HD3	1.62	0.80
1:A:68:GLY:HA3	15:A:2050:HOH:O	1.85	0.77
1:A:42:ASN:HB2	1:A:85:GLN:OE1	1.86	0.76
1:B:43:GLU:HG3	1:B:86:ASN:HB2	1.70	0.73

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	917/942 (97%)	894 (98%)	23 (2%)	0	100	100
1	B	916/942 (97%)	889 (97%)	26 (3%)	1 (0%)	55	76
All	All	1833/1884 (97%)	1783 (97%)	49 (3%)	1 (0%)	55	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	798	ILE

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	778/811 (96%)	763 (98%)	15 (2%)	62	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	774/811 (95%)	760 (98%)	14 (2%)	64	86
All	All	1552/1622 (96%)	1523 (98%)	29 (2%)	62	85

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	860	SER
1	B	70	SER
1	B	699	ARG
1	A	880	THR
1	B	99	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

65 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	0.29	0	15,19,21	0.49	0
2	NAG	A	1944	2	14,14,15	0.37	0	15,19,21	0.83	0
2	BMA	A	1945	2	11,11,12	0.52	0	13,15,17	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	A	1946	2	11,11,12	0.45	0	13,15,17	0.98	1 (7%)
2	MAN	A	1947	2	11,11,12	0.52	0	13,15,17	0.61	0
2	MAN	A	1948	2	11,11,12	0.74	0	14,15,17	1.31	2 (14%)
3	NAG	A	1949	1,3	14,14,15	0.41	0	15,19,21	2.74	4 (26%)
3	NAG	A	1950	3	14,14,15	0.72	0	15,19,21	1.01	1 (6%)
3	MAN	A	1951	3	11,11,12	0.58	0	13,15,17	1.25	1 (7%)
5	NAG	A	1954	1,5	14,14,15	0.56	0	15,19,21	0.85	0
5	NAG	A	1955	5	14,14,15	0.60	0	15,19,21	0.74	0
6	NAG	A	1956	1,6	14,14,15	0.42	0	15,19,21	0.83	1 (6%)
6	NAG	A	1957	6	14,14,15	0.96	1 (7%)	15,19,21	1.85	2 (13%)
6	BMA	A	1958	6	11,11,12	0.39	0	13,15,17	1.66	1 (7%)
6	BMA	A	1959	6	11,11,12	0.34	0	13,15,17	1.72	3 (23%)
6	MAN	A	1960	6	11,11,12	0.24	0	13,15,17	1.17	1 (7%)
6	MAN	A	1961	6	11,11,12	0.50	0	13,15,17	0.76	1 (7%)
6	MAN	A	1962	6	11,11,12	0.86	1 (9%)	13,15,17	2.76	1 (7%)
6	MAN	A	1963	6	11,11,12	0.30	0	13,15,17	0.92	1 (7%)
6	MAN	A	1964	6	11,11,12	0.57	0	13,15,17	0.83	1 (7%)
6	MAN	A	1965	6	11,11,12	0.73	0	13,15,17	2.09	3 (23%)
6	MAN	A	1966	6	11,11,12	0.42	0	13,15,17	0.74	0
7	NAG	A	1968	1,7	14,14,15	0.65	0	15,19,21	0.82	1 (6%)
7	NAG	A	1969	7	14,14,15	0.90	0	15,19,21	1.33	2 (13%)
7	MAN	A	1970	7	11,11,12	0.49	0	13,15,17	1.52	2 (15%)
7	MAN	A	1971	7	11,11,12	0.41	0	13,15,17	1.28	1 (7%)
7	MAN	A	1972	7	11,11,12	0.41	0	13,15,17	1.16	1 (7%)
7	MAN	A	1973	7	11,11,12	0.89	0	13,15,17	0.99	1 (7%)
7	MAN	A	1974	7	11,11,12	0.62	0	13,15,17	0.80	1 (7%)
7	MAN	A	1975	7	11,11,12	0.50	0	13,15,17	0.98	1 (7%)
5	NAG	A	1976	1,5	14,14,15	0.50	0	15,19,21	0.76	0
5	NAG	A	1977	5	14,14,15	1.02	1 (7%)	16,19,21	2.67	3 (18%)
12	NAG	B	1943	1,12	14,14,15	0.60	0	15,19,21	0.57	0
12	NAG	B	1944	12	14,14,15	0.41	0	15,19,21	0.64	0
12	MAN	B	1945	12	11,11,12	0.72	0	13,15,17	1.38	2 (15%)
12	MAN	B	1946	12	11,11,12	0.41	0	13,15,17	0.90	1 (7%)
12	MAN	B	1947	12	11,11,12	0.46	0	13,15,17	1.36	1 (7%)
12	MAN	B	1948	12	11,11,12	0.60	0	13,15,17	1.67	2 (15%)
12	MAN	B	1949	12	11,11,12	0.82	0	13,15,17	1.07	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	MAN	B	1950	12	11,11,12	0.60	0	13,15,17	0.90	1 (7%)
12	MAN	B	1951	12	11,11,12	0.68	0	13,15,17	0.87	1 (7%)
2	NAG	B	1952	1,2	14,14,15	0.27	0	15,19,21	0.69	0
2	NAG	B	1953	2	14,14,15	0.50	0	15,19,21	1.06	0
2	BMA	B	1954	2	11,11,12	0.41	0	13,15,17	0.76	0
2	MAN	B	1955	2	11,11,12	0.23	0	13,15,17	1.11	1 (7%)
2	MAN	B	1956	2	11,11,12	0.42	0	13,15,17	0.68	0
2	MAN	B	1957	2	10,10,12	1.11	1 (10%)	10,13,17	1.49	2 (20%)
6	NAG	B	1958	1,6	14,14,15	0.47	0	15,19,21	0.88	1 (6%)
6	NAG	B	1959	6	14,14,15	0.29	0	15,19,21	0.63	0
6	BMA	B	1960	6	11,11,12	0.52	0	13,15,17	1.93	1 (7%)
6	BMA	B	1961	6	11,11,12	0.54	0	13,15,17	1.67	2 (15%)
6	MAN	B	1962	6	11,11,12	0.22	0	13,15,17	1.00	1 (7%)
6	MAN	B	1963	6	11,11,12	0.39	0	13,15,17	0.88	1 (7%)
6	MAN	B	1964	6	11,11,12	0.59	0	13,15,17	1.84	2 (15%)
6	MAN	B	1965	6	11,11,12	0.34	0	13,15,17	0.67	0
6	MAN	B	1966	6	11,11,12	0.48	0	13,15,17	0.83	1 (7%)
6	MAN	B	1967	6	11,11,12	0.66	0	13,15,17	0.54	0
6	MAN	B	1968	6	11,11,12	0.39	0	13,15,17	0.91	1 (7%)
5	NAG	B	1972	1,5	14,14,15	0.59	0	15,19,21	0.77	0
5	NAG	B	1973	5	14,14,15	0.91	1 (7%)	16,19,21	2.57	3 (18%)
3	NAG	B	1975	1,3	14,14,15	0.26	0	15,19,21	1.05	1 (6%)
3	NAG	B	1976	3	14,14,15	0.72	0	15,19,21	0.74	0
3	MAN	B	1977	3	11,11,12	0.59	0	13,15,17	1.28	2 (15%)
5	NAG	B	1978	1,5	14,14,15	0.94	0	15,19,21	1.74	4 (26%)
5	NAG	B	1979	5	14,14,15	0.69	0	15,19,21	0.69	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
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
2	MAN	A	1946	2	-	0/2/19/22	0/1/1/1
2	MAN	A	1947	2	-	0/2/19/22	0/1/1/1
2	MAN	A	1948	2	-	0/2/18/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1949	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1950	3	-	0/6/23/26	0/1/1/1
3	MAN	A	1951	3	-	0/2/19/22	1/1/1/1
5	NAG	A	1954	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1955	5	-	0/6/23/26	0/1/1/1
6	NAG	A	1956	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1957	6	-	0/6/23/26	0/1/1/1
6	BMA	A	1958	6	-	0/2/19/22	0/1/1/1
6	BMA	A	1959	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1960	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1961	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1962	6	-	0/2/19/22	0/1/1/1
6	MAN	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	1/1/4/5	0/2/19/22	0/1/1/1
6	MAN	A	1966	6	-	0/2/19/22	0/1/1/1
7	NAG	A	1968	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1969	7	-	0/6/23/26	0/1/1/1
7	MAN	A	1970	7	-	0/2/19/22	1/1/1/1
7	MAN	A	1971	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1972	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1973	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1974	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1975	7	-	0/2/19/22	0/1/1/1
5	NAG	A	1976	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1977	5	-	0/6/22/26	0/1/1/1
12	NAG	B	1943	1,12	-	0/6/23/26	0/1/1/1
12	NAG	B	1944	12	-	0/6/23/26	0/1/1/1
12	MAN	B	1945	12	-	0/2/19/22	1/1/1/1
12	MAN	B	1946	12	-	0/2/19/22	0/1/1/1
12	MAN	B	1947	12	-	0/2/19/22	0/1/1/1
12	MAN	B	1948	12	-	0/2/19/22	0/1/1/1
12	MAN	B	1949	12	-	0/2/19/22	0/1/1/1
12	MAN	B	1950	12	-	0/2/19/22	0/1/1/1
12	MAN	B	1951	12	-	0/2/19/22	0/1/1/1
2	NAG	B	1952	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1953	2	-	0/6/23/26	0/1/1/1
2	BMA	B	1954	2	-	0/2/19/22	0/1/1/1
2	MAN	B	1955	2	-	0/2/19/22	0/1/1/1
2	MAN	B	1956	2	-	0/2/19/22	0/1/1/1
2	MAN	B	1957	2	-	0/2/16/22	0/1/1/1
6	NAG	B	1958	1,6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	1959	6	-	0/6/23/26	0/1/1/1
6	BMA	B	1960	6	-	0/2/19/22	0/1/1/1
6	BMA	B	1961	6	-	0/2/19/22	0/1/1/1
6	MAN	B	1962	6	-	0/2/19/22	0/1/1/1
6	MAN	B	1963	6	-	0/2/19/22	0/1/1/1
6	MAN	B	1964	6	-	0/2/19/22	0/1/1/1
6	MAN	B	1965	6	-	0/2/19/22	0/1/1/1
6	MAN	B	1966	6	-	0/2/19/22	0/1/1/1
6	MAN	B	1967	6	-	0/2/19/22	0/1/1/1
6	MAN	B	1968	6	-	0/2/19/22	0/1/1/1
5	NAG	B	1972	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1973	5	-	0/6/22/26	0/1/1/1
3	NAG	B	1975	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1976	3	-	0/6/23/26	0/1/1/1
3	MAN	B	1977	3	-	0/2/19/22	1/1/1/1
5	NAG	B	1978	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1979	5	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1957	NAG	O5-C1	-2.30	1.40	1.43
6	A	1962	MAN	O3-C3	-2.13	1.38	1.43
2	B	1957	MAN	O5-C1	2.12	1.49	1.44
5	B	1973	NAG	C1-C2	2.90	1.56	1.52
5	A	1977	NAG	C1-C2	3.25	1.56	1.52

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1962	MAN	O3-C3-C4	-9.50	89.69	110.36
5	A	1977	NAG	C1-C2-N2	-8.74	100.60	110.73
5	B	1973	NAG	C1-C2-N2	-8.50	100.88	110.73
6	A	1965	MAN	O5-C1-C2	-6.44	100.71	110.79
6	A	1957	NAG	O5-C1-C2	-5.24	104.18	111.47

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	1965	MAN	C1

There are no torsion outliers.

All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1977	MAN	C1-C2-C3-C4-C5-O5
12	B	1945	MAN	C1-C2-C3-C4-C5-O5
3	A	1951	MAN	C1-C2-C3-C4-C5-O5
7	A	1970	MAN	C1-C2-C3-C4-C5-O5

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1949	NAG	1	0
3	A	1951	MAN	1	0
5	A	1977	NAG	1	0
2	B	1952	NAG	1	0
2	B	1953	NAG	2	0
5	B	1973	NAG	1	0
3	B	1975	NAG	1	0
5	B	1978	NAG	1	0

5.6 Ligand geometry [i](#)

Of 47 ligands modelled in this entry, 33 are monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	1952	1	14,14,15	0.53	0	15,19,21	0.88	1 (6%)
4	NAG	A	1953	1	14,14,15	0.42	0	15,19,21	0.80	1 (6%)
4	NAG	A	1967	1	14,14,15	0.62	0	15,19,21	0.65	0
4	NAG	A	1978	1	14,14,15	0.55	0	15,19,21	0.56	0
4	NAG	A	1979	1	14,14,15	0.37	0	15,19,21	0.81	1 (6%)
10	1PE	A	1997	-	8,8,15	0.36	0	7,7,14	0.70	0
11	PE4	A	1998	-	9,9,23	0.51	0	8,8,22	0.52	0
4	NAG	B	1969	1	14,14,15	0.44	0	15,19,21	0.76	0
4	NAG	B	1970	1	14,14,15	0.58	0	15,19,21	0.73	0
4	NAG	B	1971	1	14,14,15	0.60	0	15,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	1974	1	14,14,15	0.66	1 (7%)	15,19,21	0.92	1 (6%)
4	NAG	B	1980	1	14,14,15	0.47	0	15,19,21	1.19	1 (6%)
10	1PE	B	1993	-	8,8,15	0.37	0	7,7,14	0.81	0
11	PE4	B	1995	-	15,15,23	0.50	0	14,14,22	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1952	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1953	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1967	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1978	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1979	1	-	0/6/23/26	0/1/1/1
10	1PE	A	1997	-	-	0/6/6/13	0/0/0/0
11	PE4	A	1998	-	-	0/7/7/21	0/0/0/0
4	NAG	B	1969	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1970	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1971	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1974	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1980	1	-	0/6/23/26	0/1/1/1
10	1PE	B	1993	-	-	0/6/6/13	0/0/0/0
11	PE4	B	1995	-	-	0/13/13/21	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1974	NAG	C1-C2	2.15	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1980	NAG	C2-N2-C7	-2.67	119.04	122.94
4	A	1979	NAG	C2-N2-C7	-2.10	119.88	122.94
4	A	1953	NAG	C1-O5-C5	2.35	115.41	112.17
4	A	1952	NAG	C1-O5-C5	2.74	115.94	112.17
4	B	1974	NAG	C1-O5-C5	3.12	116.47	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1998	PE4	2	0
11	B	1995	PE4	2	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	917/942 (97%)	0.04	3 (0%)	93 94	33, 51, 85, 114	1 (0%)
1	B	917/942 (97%)	-0.01	1 (0%)	95 95	31, 48, 76, 113	0
All	All	1834/1884 (97%)	0.01	4 (0%)	94 95	31, 49, 81, 114	1 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	333	ALA	3.0
1	B	559	TYR	2.3
1	A	326	ILE	2.1
1	A	334	GLY	2.0

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
12	MAN	B	1951	11/12	0.87	0.39	5.67	59,66,69,71	0
7	MAN	A	1975	11/12	0.87	0.24	4.70	60,63,66,68	0
6	MAN	B	1963	11/12	0.94	0.18	1.35	55,60,64,64	0
6	MAN	A	1961	11/12	0.93	0.20	1.27	57,62,63,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MAN	B	1965	11/12	0.97	0.16	0.87	43,44,49,52	0
2	NAG	B	1953	14/15	0.97	0.17	0.12	38,43,48,53	0
2	NAG	A	1943	14/15	0.97	0.17	0.08	42,44,50,51	0
6	BMA	B	1961	11/12	0.94	0.16	-0.12	40,46,51,52	0
2	NAG	B	1952	14/15	0.98	0.17	-0.19	41,44,46,46	0
6	NAG	B	1958	14/15	0.98	0.15	-0.22	42,44,46,47	0
2	NAG	A	1944	14/15	0.96	0.15	-0.38	43,45,49,53	0
12	NAG	B	1943	14/15	0.96	0.14	-0.64	39,47,52,52	0
6	NAG	A	1957	14/15	0.97	0.15	-0.66	44,47,58,59	0
6	NAG	A	1956	14/15	0.98	0.14	-0.79	44,47,48,49	0
3	NAG	A	1949	14/15	0.97	0.14	-0.85	40,42,49,50	0
2	MAN	B	1956	11/12	0.97	0.14	-0.89	40,45,48,49	0
6	BMA	A	1959	11/12	0.92	0.14	-1.03	44,45,51,51	0
6	NAG	B	1959	14/15	0.98	0.14	-1.11	40,42,46,46	0
2	MAN	B	1955	11/12	0.97	0.14	-1.28	41,44,48,48	0
5	NAG	B	1978	14/15	0.96	0.12	-1.39	37,44,52,59	0
5	NAG	A	1954	14/15	0.95	0.12	-1.72	39,43,51,54	0
7	NAG	A	1968	14/15	0.96	0.12	-1.88	43,53,59,61	0
2	MAN	A	1947	11/12	0.95	0.12	-2.00	40,50,52,55	0
2	MAN	A	1946	11/12	0.97	0.13	-2.14	38,47,49,50	0
6	MAN	A	1963	11/12	0.98	0.12	-2.23	47,49,51,52	0
6	MAN	A	1964	11/12	0.95	0.12	-2.69	46,50,51,52	0
3	NAG	B	1975	14/15	0.97	0.13	-3.19	37,39,42,43	0
6	MAN	B	1966	11/12	0.96	0.12	-3.95	48,51,54,55	0
12	NAG	B	1944	14/15	0.97	0.13	-	47,55,58,63	0
5	NAG	A	1977	14/15	0.83	0.17	-	58,67,69,73	0
7	MAN	A	1970	11/12	0.87	0.15	-	61,62,64,67	0
7	MAN	A	1971	11/12	0.90	0.15	-	62,64,66,67	0
12	MAN	B	1950	11/12	0.90	0.21	-	58,62,66,67	0
12	MAN	B	1948	11/12	0.61	0.30	-	71,74,77,77	11
7	MAN	A	1973	11/12	0.85	0.21	-	61,65,67,67	0
12	MAN	B	1945	11/12	0.90	0.17	-	57,61,64,68	0
6	MAN	A	1965	11/12	0.91	0.15	-	53,55,60,61	0
2	MAN	B	1957	10/12	0.83	0.15	-	24,26,26,27	0
6	MAN	B	1962	11/12	0.97	0.12	-	44,49,52,53	0
5	NAG	A	1955	14/15	0.90	0.13	-	53,58,68,72	0
5	NAG	B	1972	14/15	0.94	0.15	-	46,50,53,55	0
6	BMA	A	1958	11/12	0.92	0.17	-	47,47,50,51	0
7	MAN	A	1972	11/12	0.91	0.14	-	55,61,68,71	0
6	MAN	A	1966	11/12	0.95	0.13	-	56,57,59,59	0
3	NAG	B	1976	14/15	0.97	0.13	-	39,44,50,50	0
2	BMA	B	1954	11/12	0.96	0.11	-	43,47,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	A	1950	14/15	0.97	0.12	-	38,46,51,53	0
6	MAN	B	1968	11/12	0.96	0.12	-	49,52,54,54	0
3	MAN	A	1951	11/12	0.88	0.14	-	52,56,62,63	0
6	BMA	B	1960	11/12	0.95	0.16	-	44,46,50,50	0
7	MAN	A	1974	11/12	0.93	0.16	-	57,58,62,64	0
6	MAN	B	1967	11/12	0.97	0.13	-	48,50,55,56	0
5	NAG	B	1979	14/15	0.91	0.13	-	49,55,63,63	0
2	BMA	A	1945	11/12	0.97	0.11	-	46,50,57,61	0
12	MAN	B	1949	11/12	0.91	0.27	-	63,67,68,68	0
5	NAG	A	1976	14/15	0.96	0.16	-	46,50,54,56	0
5	NAG	B	1973	14/15	0.79	0.19	-	59,66,70,71	0
12	MAN	B	1946	11/12	0.92	0.16	-	61,63,67,67	0
7	NAG	A	1969	14/15	0.94	0.14	-	52,56,60,65	0
12	MAN	B	1947	11/12	0.89	0.15	-	55,61,69,73	0
2	MAN	A	1948	11/12	0.88	0.13	-	65,67,70,71	0
3	MAN	B	1977	11/12	0.89	0.15	-	51,56,61,62	0
6	MAN	B	1964	11/12	0.97	0.12	-	45,47,49,51	0
6	MAN	A	1962	11/12	0.93	0.13	-	50,52,55,59	0
6	MAN	A	1960	11/12	0.95	0.14	-	47,50,51,54	0

6.4 Ligands [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(\AA^2)	Q<0.9
11	PE4	A	1998	10/24	0.91	0.32	10.80	58,63,65,67	0
11	PE4	B	1995	16/24	0.92	0.28	7.36	56,62,69,71	0
9	NA	B	1992	1/1	0.91	0.23	5.78	57,57,57,57	0
9	NA	A	1996	1/1	0.90	0.23	5.67	55,55,55,55	0
4	NAG	A	1979	14/15	0.76	0.25	2.05	24,25,26,27	14
4	NAG	B	1980	14/15	0.82	0.24	1.70	24,25,26,27	14
4	NAG	B	1970	14/15	0.87	0.16	0.69	54,57,65,65	0
4	NAG	B	1969	14/15	0.88	0.19	0.64	63,66,69,70	0
4	NAG	A	1953	14/15	0.91	0.18	0.64	62,65,68,70	0
4	NAG	A	1978	14/15	0.90	0.15	0.48	51,60,63,65	0
4	NAG	B	1971	14/15	0.94	0.13	-0.92	39,44,50,50	0
4	NAG	A	1967	14/15	0.94	0.13	-1.43	40,46,49,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
14	CA	B	1996	1/1	0.97	0.07	-7.93	54,54,54,54	0
8	CD	A	1983	1/1	0.73	0.05	-	141,141,141,141	0
8	CD	A	1993	1/1	1.00	0.15	-	39,39,39,39	0
8	CD	A	2000	1/1	0.94	0.04	-	120,120,120,120	0
8	CD	B	1983	1/1	0.94	0.06	-	94,94,94,94	0
8	CD	A	1990	1/1	0.99	0.08	-	58,58,58,58	1
8	CD	B	1987	1/1	0.94	0.12	-	56,56,56,56	1
8	CD	B	1986	1/1	0.93	0.13	-	35,35,35,35	1
8	CD	A	1991	1/1	0.98	0.05	-	63,63,63,63	1
10	1PE	A	1997	9/16	0.94	0.15	-	51,52,53,53	0
8	CD	A	1987	1/1	1.00	0.14	-	39,39,39,39	0
8	CD	B	1982	1/1	0.97	0.04	-	127,127,127,127	0
8	CD	B	2000	1/1	0.97	0.03	-	114,114,114,114	0
8	CD	B	1991	1/1	0.95	0.11	-	79,79,79,79	0
8	CD	A	1994	1/1	0.97	0.10	-	102,102,102,102	0
4	NAG	B	1974	14/15	0.90	0.17	-	59,62,64,70	0
8	CD	B	1988	1/1	0.99	0.07	-	83,83,83,83	1
9	NA	A	1995	1/1	0.91	0.33	-	48,48,48,48	0
8	CD	A	1981	1/1	0.95	0.09	-	82,82,82,82	1
8	CD	A	1982	1/1	0.94	0.11	-	73,73,73,73	1
4	NAG	A	1952	14/15	0.92	0.16	-	65,68,71,71	0
8	CD	A	1986	1/1	1.00	0.15	-	40,40,40,40	0
8	CD	B	1984	1/1	0.99	0.16	-	54,54,54,54	0
8	CD	B	1985	1/1	0.99	0.12	-	59,59,59,59	0
8	CD	A	1985	1/1	1.00	0.15	-	41,41,41,41	0
8	CD	A	1980	1/1	0.94	0.24	-	54,54,54,54	1
8	CD	A	1992	1/1	0.99	0.16	-	47,47,47,47	0
8	CD	A	1984	1/1	0.96	0.06	-	94,94,94,94	0
8	CD	B	1990	1/1	1.00	0.16	-	47,47,47,47	0
10	1PE	B	1993	9/16	0.95	0.15	-	51,53,54,54	0
13	CL	B	1994	1/1	0.95	0.17	-	53,53,53,53	0
8	CD	A	1989	1/1	0.98	0.17	-	47,47,47,47	1
8	CD	B	1981	1/1	0.97	0.22	-	58,58,58,58	1
8	CD	A	1988	1/1	0.99	0.16	-	55,55,55,55	0
8	CD	B	1989	1/1	0.97	0.13	-	95,95,95,95	0

6.5 Other polymers

There are no such residues in this entry.