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wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 16, 2024 – 09:25 AM EST

PDB ID	:	3H5C
Title	:	X-Ray Structure of Protein Z-Protein Z Inhibitor Complex
Authors	:	Dementiev, A.A.; Huang, X.; Olson, S.T.; Gettins, P.G.W.
Deposited on	:	2009-04-21
Resolution	:	3.26 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.26 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.
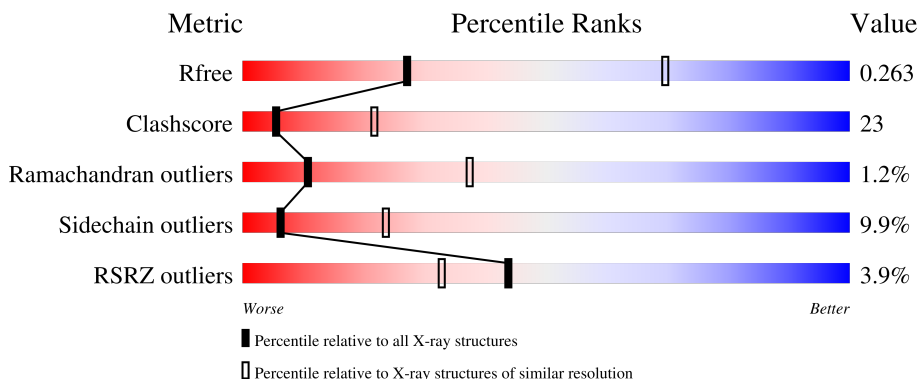
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1482 (3.30-3.22)
Clashscore	180529	1546 (3.30-3.22)
Ramachandran outliers	177936	1536 (3.30-3.22)
Sidechain outliers	177891	1535 (3.30-3.22)
RSRZ outliers	164620	1483 (3.30-3.22)

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% 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	423	3% / 58% / 29% / • / 9%
2	B	317	4% / 54% / 39% / 5% / •

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
4	BGC	B	401	-	-	X	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 5357 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 Protein Z-dependent protease inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	0	0
			2930	1891	497	521	21			

- Molecule 2 is a protein called Vitamin K-dependent protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	312	Total	C	N	O	S	0	0	0
			2313	1436	413	439	25			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
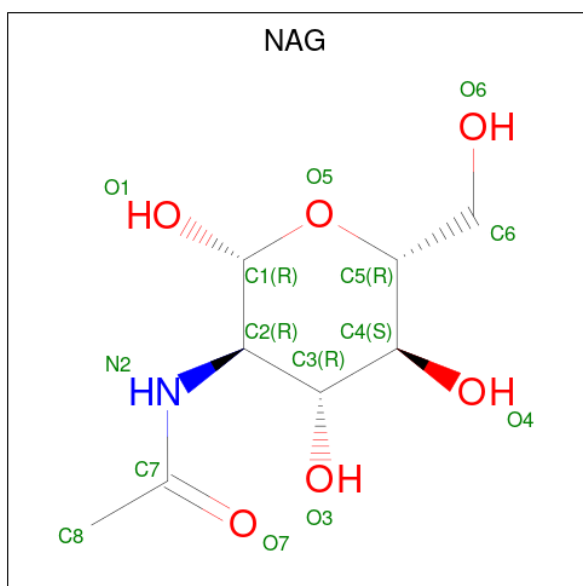
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 4 is beta-D-glucopyranose (three-letter code: BGC) (formula: $C_6H_{12}O_6$).

BGC
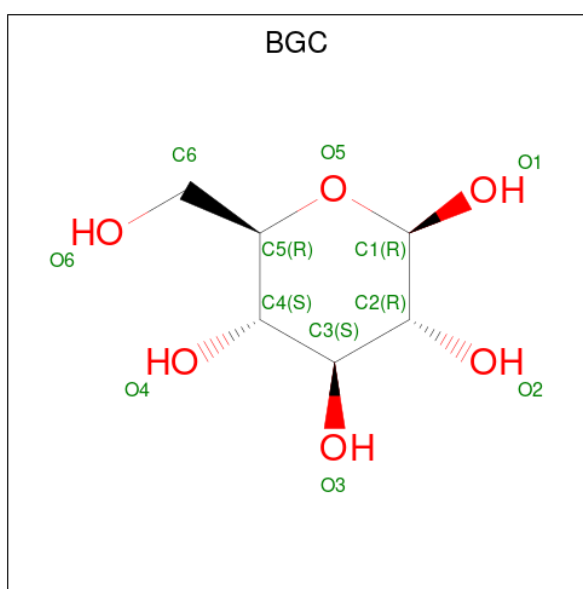
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 11	C 6	O 5	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total 10	O 10	0	0
5	B	9	Total 9	O 9	0	0

3 Residue-property plots ⓘ

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 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: Protein Z-dependent protease inhibitor

Chain A:
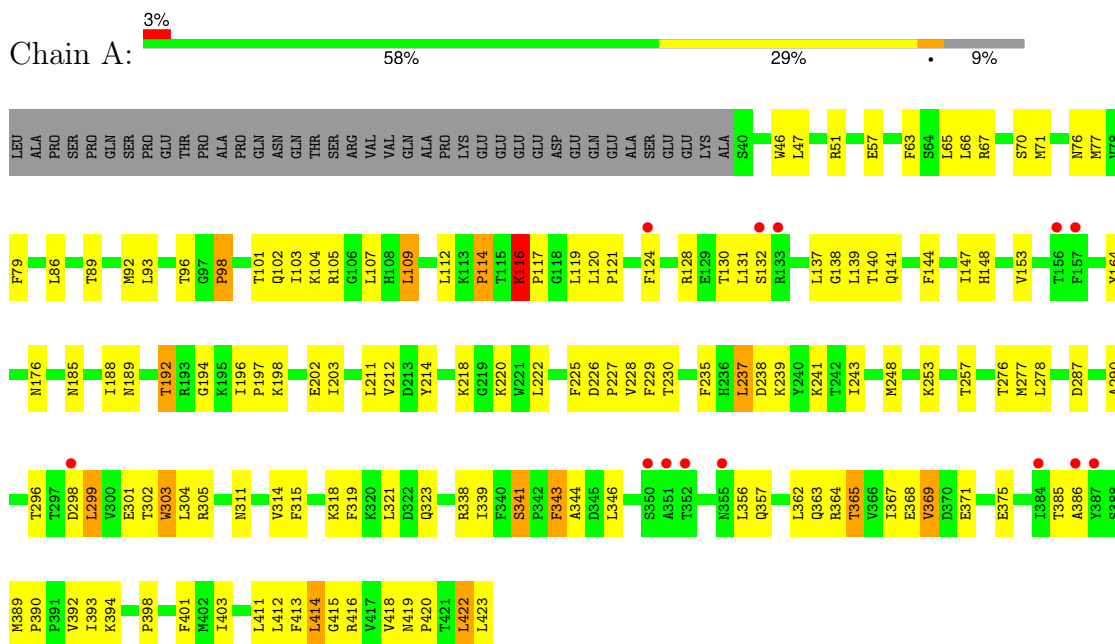
• Molecule 2: Vitamin K-dependent protein Z

Chain B:
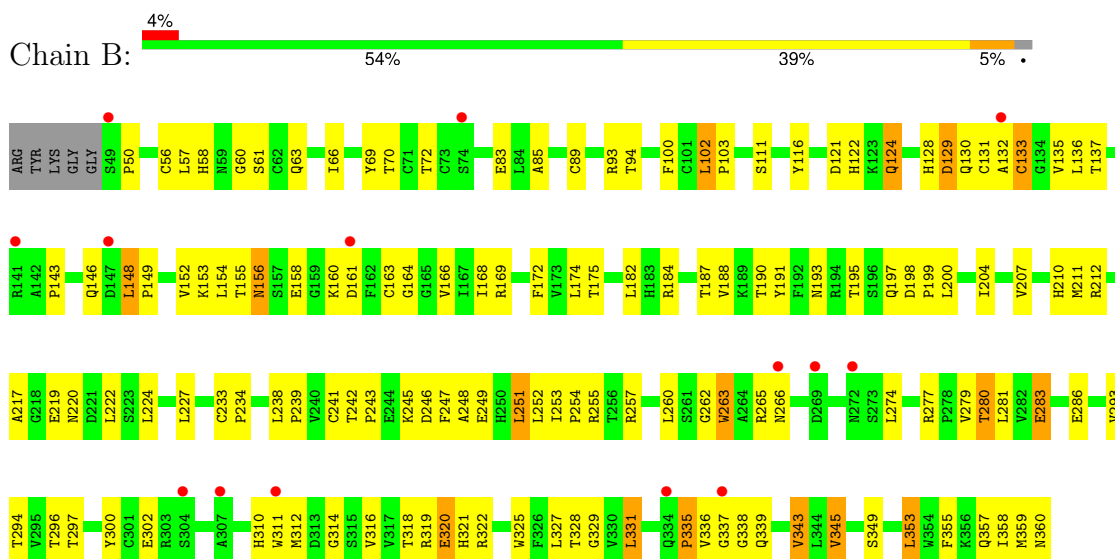
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	119.93Å 119.93Å 347.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.58 – 3.26 44.58 – 3.26	Depositor EDS
% Data completeness (in resolution range)	97.8 (44.58-3.26) 97.7 (44.58-3.26)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.201 , 0.269 0.214 , 0.263	Depositor DCC
R_{free} test set	1703 reflections (7.25%)	wwPDB-VP
Wilson B-factor (Å^2)	83.6	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 73.1	EDS
L-test for twinning[2]	$< |L| > = 0.45, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5357	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: BGC, NAG

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	0.27	0/2994	0.50	0/4059
2	B	0.27	0/2364	0.54	0/3219
All	All	0.27	0/5358	0.52	0/7278

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 ⓘ

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	2930	0	2845	125	0
2	B	2313	0	2098	123	0
3	A	28	0	26	0	0
3	B	56	0	52	0	0
4	B	11	0	10	8	0
5	A	10	0	0	2	0
5	B	9	0	0	0	0
All	All	5357	0	5031	242	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 23.

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The worst 5 of 242 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:A:116:LYS:HB3	1:A:117:PRO:CD	1.53	1.37
1:A:116:LYS:CB	1:A:117:PRO:CD	2.22	1.15
1:A:116:LYS:CG	1:A:117:PRO:HD3	1.75	1.14
1:A:422:LEU:O	1:A:423:LEU:HB2	1.48	1.13
1:A:116:LYS:HB3	1:A:117:PRO:HD2	1.06	1.04

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	382/423 (90%)	326 (85%)	51 (13%)	5 (1%)	10	35
2	B	310/317 (98%)	253 (82%)	54 (17%)	3 (1%)	13	41
All	All	692/740 (94%)	579 (84%)	105 (15%)	8 (1%)	11	37

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	LYS
2	B	335	PRO
1	A	197	PRO
2	B	143	PRO
1	A	114	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	298/377 (79%)	274 (92%)	24 (8%)	9	30
2	B	239/275 (87%)	210 (88%)	29 (12%)	4	16
All	All	537/652 (82%)	484 (90%)	53 (10%)	6	23

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	124	GLN
2	B	184	ARG
2	B	331	LEU
2	B	129	ASP
2	B	156	ASN

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

Mol	Chain	Res	Type
2	B	156	ASN
2	B	128	HIS
1	A	323	GLN
1	A	272	GLN
2	B	124	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 ligands 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	#$|Z| > 2$
3	NAG	B	402	2	14,14,15	0.53	0	17,19,21	0.64	0
3	NAG	B	404	2	14,14,15	0.46	0	17,19,21	1.37	3 (17%)
3	NAG	B	403	2	14,14,15	0.49	0	17,19,21	1.12	1 (5%)
3	NAG	A	501	1	14,14,15	0.51	0	17,19,21	0.76	1 (5%)
4	BGC	B	401	-	11,11,12	0.63	0	15,15,17	0.67	0
3	NAG	A	502	1	14,14,15	0.51	0	17,19,21	1.28	2 (11%)
3	NAG	B	405	2	14,14,15	0.48	0	17,19,21	0.81	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
3	NAG	B	402	2	-	1/6/23/26	0/1/1/1
3	NAG	B	404	2	-	1/6/23/26	0/1/1/1
3	NAG	B	403	2	-	1/6/23/26	0/1/1/1
3	NAG	A	501	1	-	1/6/23/26	0/1/1/1
4	BGC	B	401	-	-	0/2/19/22	0/1/1/1
3	NAG	A	502	1	-	2/6/23/26	0/1/1/1
3	NAG	B	405	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	NAG	C2-N2-C7	3.50	127.59	122.90
3	B	404	NAG	C2-N2-C7	3.21	127.20	122.90
3	B	403	NAG	C2-N2-C7	2.99	126.91	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	404	NAG	C1-O5-C5	2.61	115.69	112.19
3	B	404	NAG	C1-C2-N2	2.50	114.37	110.43

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	NAG	C1-C2-N2-C7
3	B	403	NAG	C1-C2-N2-C7
3	B	404	NAG	C1-C2-N2-C7
3	B	405	NAG	C8-C7-N2-C2
3	B	405	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	401	BGC	8	0

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	384/423 (90%)	-0.01	13 (3%)	48	36	54, 76, 139, 164	0
2	B	312/317 (98%)	0.17	14 (4%)	39	29	53, 89, 148, 200	0
All	All	696/740 (94%)	0.07	27 (3%)	44	33	53, 82, 145, 200	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	ARG	4.3
2	B	334	GLN	3.8
2	B	147	ASP	3.6
2	B	49	SER	3.5
1	A	124	PHE	3.4

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 ⓘ

There are no monosaccharides in this entry.

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. 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	B-factors(Å^2)	Q<0.9
3	NAG	B	402	14/15	0.06	0.16	155,180,189,192	0
3	NAG	B	405	14/15	0.39	0.14	144,156,160,162	0
3	NAG	A	501	14/15	0.57	0.13	149,159,163,163	0
4	BGC	B	401	11/12	0.62	0.13	147,156,162,163	0
3	NAG	B	403	14/15	0.65	0.13	121,135,141,141	0
3	NAG	A	502	14/15	0.66	0.14	119,127,138,138	0
3	NAG	B	404	14/15	0.66	0.13	131,146,157,158	0

6.5 Other polymers ⓘ

There are no such residues in this entry.