wwPDB X-ray Structure Validation Summary Report (i)

Dec 5, 2023 – 12:53 PM JST

PDB ID	:	8HPY
Title	:	Crystal structure of human LGI1-ADAM22 complex
Authors	:	Liu, H.; Xu, F.
Deposited on	:	2022-12-13
Resolution	:	5.87 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 (1)) were used in the production of this report:

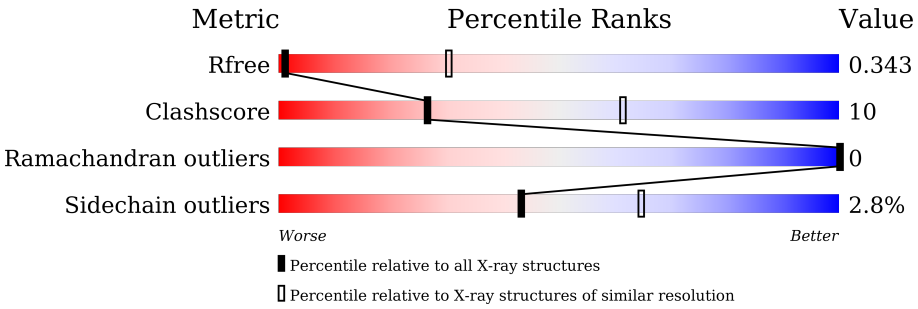
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 5.87 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}	130704	1015 (7.88-3.86)
Clashscore	141614	1041 (7.82-3.90)
Ramachandran outliers	138981	1010 (7.88-3.86)
Sidechain outliers	138945	1013 (7.94-3.82)

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%

Mol	Chain	Length	Quality of chain
1	A	486	77% 22% •
1	B	486	81% 17% •
2	D	526	71% 26% • •
2	E	526	75% 22% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15962 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 Disintegrin and metalloproteinase domain-containing protein 22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	0	0
			3710	2293	638	728	51			
1	B	484	Total	C	N	O	S	0	0	0
			3710	2293	638	728	51			

- Molecule 2 is a protein called Leucine-rich glioma-inactivated protein 1.

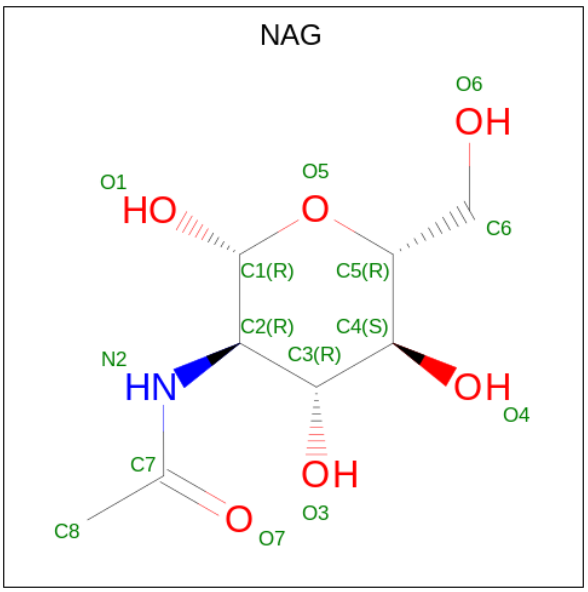
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	515	Total	C	N	O	S	0	0	0
			4183	2694	696	778	15			
2	E	515	Total	C	N	O	S	0	0	0
			4183	2694	696	778	15			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	32	HIS	-	expression tag	UNP O95970
D	33	HIS	-	expression tag	UNP O95970
D	34	HIS	-	expression tag	UNP O95970
D	35	HIS	-	expression tag	UNP O95970
D	36	HIS	-	expression tag	UNP O95970
D	37	HIS	-	expression tag	UNP O95970
D	38	HIS	-	expression tag	UNP O95970
E	32	HIS	-	expression tag	UNP O95970
E	33	HIS	-	expression tag	UNP O95970
E	34	HIS	-	expression tag	UNP O95970
E	35	HIS	-	expression tag	UNP O95970
E	36	HIS	-	expression tag	UNP O95970
E	37	HIS	-	expression tag	UNP O95970
E	38	HIS	-	expression tag	UNP O95970

- 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 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	E	1	Total C N O 14 8 1 5	0	0
3	E	1	Total C N O 14 8 1 5	0	0
3	E	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

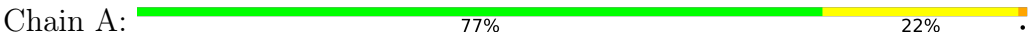
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Ca 3 3	0	0
4	D	1	Total Ca 1 1	0	0
4	B	3	Total Ca 3 3	0	0
4	E	1	Total Ca 1 1	0	0

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.

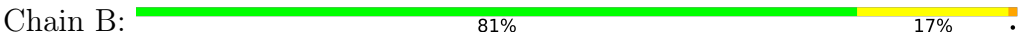
• Molecule 1: Disintegrin and metalloproteinase domain-containing protein 22

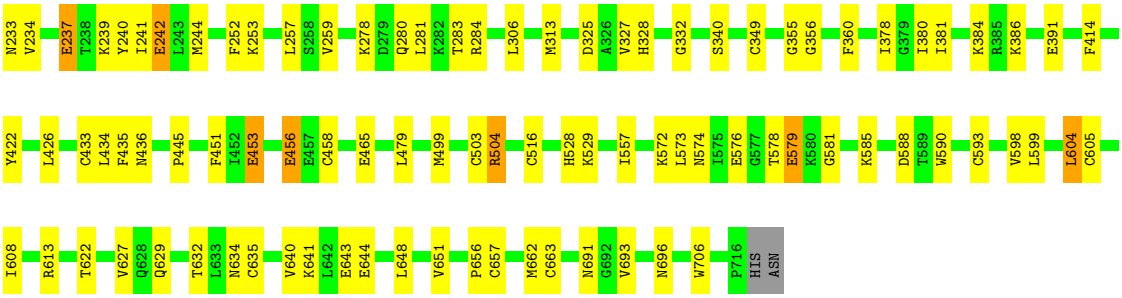
Chain A:



• Molecule 1: Disintegrin and metalloproteinase domain-containing protein 22

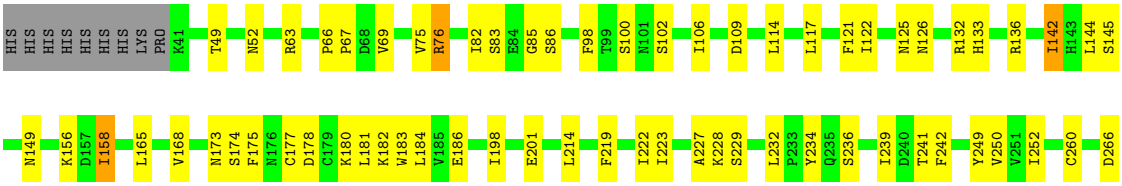
Chain B:

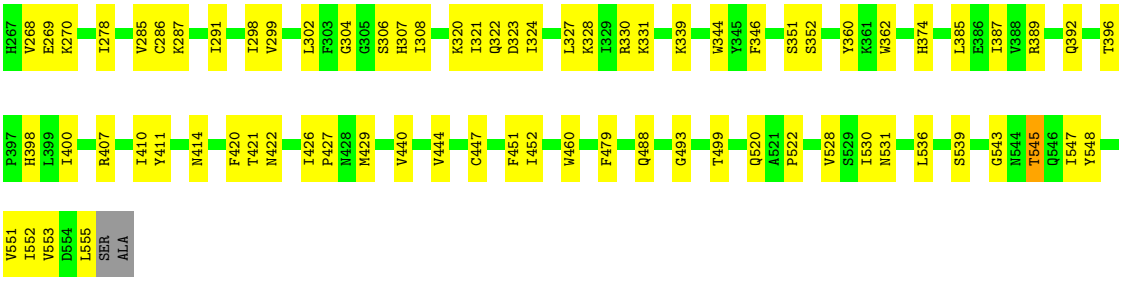




• Molecule 2: Leucine-rich glioma-inactivated protein 1

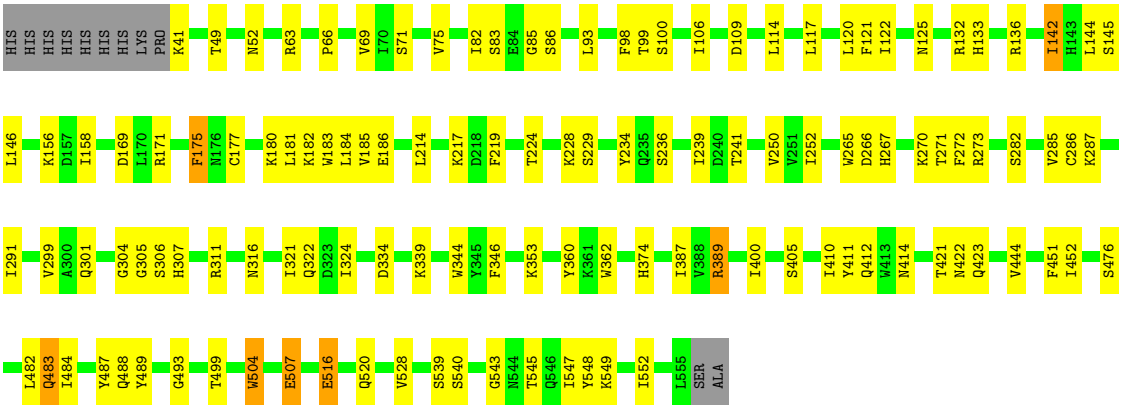
Chain D:





• Molecule 2: Leucine-rich glioma-inactivated protein 1

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α, β, γ	280.34Å 280.34Å 280.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.08 – 5.87 48.08 – 5.87	Depositor EDS
% Data completeness (in resolution range)	97.7 (48.08-5.87) 98.5 (48.08-5.87)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.33 (at 5.73Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.303 , 0.343 0.303 , 0.343	Depositor DCC
R_{free} test set	496 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	283.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 432.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.54$, $< L^2 > = 0.38$	Xtriage
Estimated twinning fraction	0.000 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	15962	wwPDB-VP
Average B, all atoms (Å^2)	392.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: CA, 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	0.31	0/3773	0.50	0/5079
1	B	0.30	0/3773	0.51	0/5079
2	D	0.26	0/4290	0.46	0/5821
2	E	0.27	0/4290	0.47	0/5821
All	All	0.28	0/16126	0.48	0/21800

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	3710	0	3566	76	0
1	B	3710	0	3566	77	0
2	D	4183	0	4100	99	0
2	E	4183	0	4099	85	0
3	A	42	0	39	0	0
3	B	42	0	39	5	0
3	D	42	0	39	0	0
3	E	42	0	39	0	0
4	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	3	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
All	All	15962	0	15487	324	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 10.

The worst 5 of 324 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)
2:D:223:ILE:HD11	2:D:555:LEU:CD1	1.68	1.20
2:D:223:ILE:HD11	2:D:555:LEU:HD11	1.19	1.09
2:D:223:ILE:CD1	2:D:555:LEU:HD11	1.98	0.92
1:B:237:GLU:HG2	1:B:435:PHE:HE1	1.32	0.92
1:B:237:GLU:HB2	1:B:504:ARG:HH22	1.34	0.92

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	482/486 (99%)	466 (97%)	16 (3%)	0	100	100
1	B	482/486 (99%)	471 (98%)	11 (2%)	0	100	100
2	D	513/526 (98%)	485 (94%)	28 (6%)	0	100	100
2	E	513/526 (98%)	488 (95%)	25 (5%)	0	100	100
All	All	1990/2024 (98%)	1910 (96%)	80 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	418/420 (100%)	400 (96%)	18 (4%)	29	54
1	B	418/420 (100%)	405 (97%)	13 (3%)	40	62
2	D	473/483 (98%)	467 (99%)	6 (1%)	69	82
2	E	473/483 (98%)	460 (97%)	13 (3%)	44	65
All	All	1782/1806 (99%)	1732 (97%)	50 (3%)	43	65

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	456	GLU
1	B	622	THR
2	E	539	SER
1	B	465	GLU
1	B	579	GLU

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	E	550	HIS
2	E	534	ASN
2	E	485	ASN
2	E	52	ASN
2	E	488	GLN

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 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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	D	602	2	14,14,15	0.37	0	17,19,21	0.43	0
3	NAG	E	602	2	14,14,15	0.90	1 (7%)	17,19,21	0.74	1 (5%)
3	NAG	D	601	2	14,14,15	0.34	0	17,19,21	0.34	0
3	NAG	B	802	1	14,14,15	0.37	0	17,19,21	0.75	1 (5%)
3	NAG	A	803	1	14,14,15	0.70	1 (7%)	17,19,21	0.43	0
3	NAG	B	801	1	14,14,15	0.54	0	17,19,21	0.45	0
3	NAG	E	601	2	14,14,15	0.35	0	17,19,21	0.37	0
3	NAG	B	803	1	14,14,15	0.41	0	17,19,21	0.57	0
3	NAG	D	603	2	14,14,15	1.02	1 (7%)	17,19,21	0.79	1 (5%)
3	NAG	E	603	2	14,14,15	0.41	0	17,19,21	0.51	0
3	NAG	A	802	1	14,14,15	0.55	0	17,19,21	0.53	0
3	NAG	A	801	1	14,14,15	0.33	0	17,19,21	0.50	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	D	602	2	-	0/6/23/26	0/1/1/1
3	NAG	E	602	2	-	1/6/23/26	0/1/1/1
3	NAG	D	601	2	-	0/6/23/26	0/1/1/1
3	NAG	B	802	1	-	2/6/23/26	0/1/1/1
3	NAG	A	803	1	-	1/6/23/26	0/1/1/1
3	NAG	B	801	1	-	1/6/23/26	0/1/1/1
3	NAG	E	601	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	803	1	-	0/6/23/26	0/1/1/1
3	NAG	D	603	2	-	2/6/23/26	0/1/1/1
3	NAG	E	603	2	-	0/6/23/26	0/1/1/1
3	NAG	A	802	1	-	0/6/23/26	0/1/1/1
3	NAG	A	801	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	603	NAG	O5-C1	-3.64	1.37	1.43
3	E	602	NAG	O5-C1	3.22	1.48	1.43
3	A	803	NAG	O5-C1	-2.22	1.40	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	802	NAG	C1-O5-C5	2.63	115.76	112.19
3	E	602	NAG	C1-O5-C5	2.38	115.41	112.19
3	D	603	NAG	C1-O5-C5	-2.22	109.19	112.19

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	802	NAG	O5-C5-C6-O6
3	B	802	NAG	C4-C5-C6-O6
3	D	603	NAG	O5-C5-C6-O6
3	E	602	NAG	O5-C5-C6-O6
3	B	801	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	802	NAG	5	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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.