Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:02 PM GMT

PDB ID	:	1NA8
Title	:	Crystal structure of ADP-ribosylation factor binding protein GGA1
Authors	:	Lui, W.W.; Collins, B.M.; Hirst, J.; Motley, A.; Millar, C.; Schu, P.; Owen, D.J.; Robinson, M.S.
Deposited on	:	2002-11-27
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

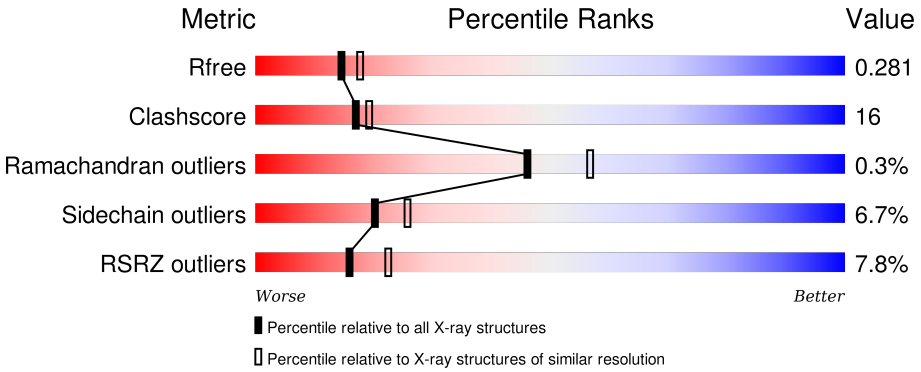
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 <=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	154	6% 68% 25% 5%
1	B	154	9% 65% 26% 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2499 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 ADP-ribosylation factor binding protein GGA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	151	Total	C	N	O	S	0	0	0
			1192	772	204	210	6			
1	B	145	Total	C	N	O	S	0	0	0
			1135	738	190	202	5			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	486	MET	-	EXPRESSION TAG	UNP Q9UJY5
A	487	HIS	-	EXPRESSION TAG	UNP Q9UJY5
A	488	HIS	-	EXPRESSION TAG	UNP Q9UJY5
A	489	HIS	-	EXPRESSION TAG	UNP Q9UJY5
A	490	HIS	-	EXPRESSION TAG	UNP Q9UJY5
A	491	HIS	-	EXPRESSION TAG	UNP Q9UJY5
A	492	HIS	-	EXPRESSION TAG	UNP Q9UJY5
A	493	MET	-	EXPRESSION TAG	UNP Q9UJY5
A	578	MET	THR	CONFLICT	UNP Q9UJY5
B	486	MET	-	EXPRESSION TAG	UNP Q9UJY5
B	487	HIS	-	EXPRESSION TAG	UNP Q9UJY5
B	488	HIS	-	EXPRESSION TAG	UNP Q9UJY5
B	489	HIS	-	EXPRESSION TAG	UNP Q9UJY5
B	490	HIS	-	EXPRESSION TAG	UNP Q9UJY5
B	491	HIS	-	EXPRESSION TAG	UNP Q9UJY5
B	492	HIS	-	EXPRESSION TAG	UNP Q9UJY5
B	493	MET	-	EXPRESSION TAG	UNP Q9UJY5
B	578	MET	THR	CONFLICT	UNP Q9UJY5

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	86	Total	O	0	0
			86	86		

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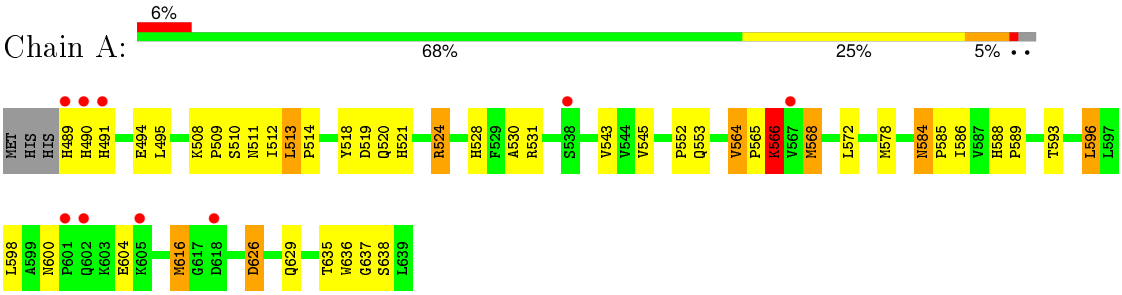
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	86	Total	O	0	0
			86	86		

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 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.

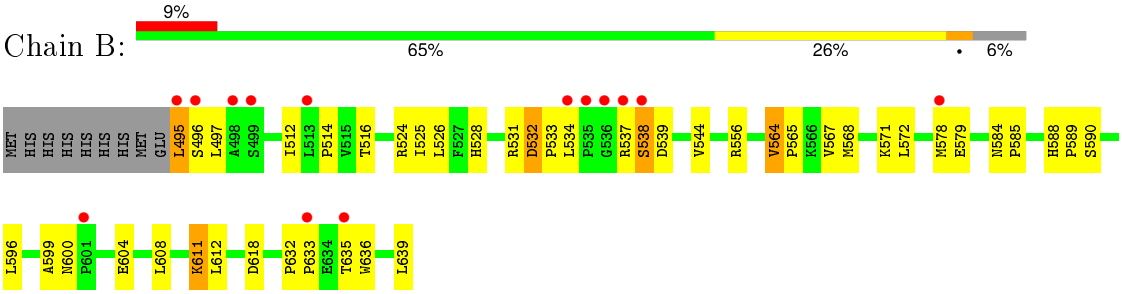
- Molecule 1: ADP-ribosylation factor binding protein GGA1

Chain A:



- Molecule 1: ADP-ribosylation factor binding protein GGA1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	65.43Å 65.43Å 142.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.30 31.89 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (15.00-2.30) 98.9 (31.89-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.92 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.216 , 0.279 0.220 , 0.281	Depositor DCC
R_{free} test set	813 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	39.3	Xtriage
Anisotropy	0.569	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 34.0	EDS
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 16192 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2499	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.74	0/1227	0.93	3/1676 (0.2%)
1	B	0.82	0/1166	0.90	3/1594 (0.2%)
All	All	0.78	0/2393	0.92	6/3270 (0.2%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	513	LEU	CA-CB-CG	6.83	131.00	115.30
1	A	626	ASP	CB-CG-OD2	6.80	124.42	118.30
1	B	532	ASP	CB-CG-OD2	6.60	124.24	118.30
1	A	519	ASP	CB-CG-OD2	5.57	123.31	118.30
1	B	618	ASP	CB-CG-OD2	5.44	123.19	118.30
1	B	578	MET	CG-SD-CE	-5.39	91.58	100.20

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	1192	0	1216	41	0
1	B	1135	0	1173	39	1
2	A	86	0	0	3	1
2	B	86	0	0	5	1
All	All	2499	0	2389	77	2

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 16.

All (77) 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:566:LYS:HD2	1:A:566:LYS:H	1.12	1.11
1:A:566:LYS:HD2	1:A:566:LYS:N	1.76	1.00
1:A:564:VAL:HG22	1:A:565:PRO:HD2	1.57	0.84
1:B:497:LEU:HD21	1:B:599:ALA:HB2	1.62	0.81
1:A:531:ARG:HH21	1:A:638:SER:HA	1.47	0.78
1:A:572:LEU:HD22	1:A:596:LEU:HD12	1.66	0.78
1:B:564:VAL:HG22	1:B:565:PRO:HD2	1.66	0.77
1:B:528:HIS:ND1	2:B:137:HOH:O	2.18	0.77
1:B:537:ARG:HG3	1:B:538:SER:H	1.51	0.74
1:B:537:ARG:HB3	1:B:539:ASP:OD1	1.89	0.73
1:A:572:LEU:HD22	1:A:596:LEU:CD1	2.21	0.70
1:B:516:THR:HA	1:B:526:LEU:HD23	1.74	0.69
1:B:516:THR:HA	1:B:526:LEU:CD2	2.26	0.65
1:A:566:LYS:CD	1:A:566:LYS:H	1.97	0.64
1:A:564:VAL:HG22	1:A:565:PRO:CD	2.26	0.64
1:A:531:ARG:NH2	1:A:638:SER:HA	2.13	0.63
1:B:572:LEU:HD21	1:B:596:LEU:HD12	1.80	0.63
1:A:572:LEU:CD2	1:A:596:LEU:CD1	2.77	0.62
1:A:578:MET:HB2	2:A:15:HOH:O	2.01	0.61
1:A:588:HIS:HD2	1:A:589:PRO:O	1.84	0.61
1:A:552:PRO:HD2	2:A:111:HOH:O	2.00	0.61
1:B:512:ILE:CD1	1:B:639:LEU:HD22	2.30	0.60
1:B:524:ARG:HD2	2:B:54:HOH:O	2.02	0.60
1:A:600:ASN:ND2	1:A:604:GLU:O	2.35	0.60
1:B:524:ARG:NH1	2:B:54:HOH:O	2.30	0.59
1:B:537:ARG:HG3	1:B:538:SER:N	2.17	0.58
1:A:568:MET:HE2	1:A:600:ASN:CG	2.25	0.57
1:A:531:ARG:HH21	1:A:638:SER:CA	2.15	0.57
1:B:537:ARG:HG2	1:B:539:ASP:OD1	2.06	0.55
1:A:511:ASN:O	1:A:512:ILE:C	2.44	0.54
1:A:524:ARG:HD2	2:A:131:HOH:O	2.07	0.54
1:A:553:GLN:HB2	1:A:616:MET:CE	2.38	0.53
1:A:491:HIS:O	1:A:495:LEU:HG	2.09	0.52
1:B:514:PRO:HB3	1:B:528:HIS:CD2	2.44	0.52
1:B:512:ILE:HD12	1:B:639:LEU:HD22	1.91	0.52
1:A:584:ASN:HD22	1:A:585:PRO:HD2	1.74	0.52
1:B:525:ILE:HD12	1:B:612:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:LEU:HD22	1:B:496:SER:O	2.11	0.50
1:A:553:GLN:HB2	1:A:616:MET:HE2	1.93	0.49
1:B:532:ASP:OD1	1:B:534:LEU:N	2.45	0.49
1:B:537:ARG:CB	1:B:539:ASP:OD1	2.60	0.48
1:A:585:PRO:CB	1:B:544:VAL:HG11	2.44	0.48
1:A:598:LEU:HD23	1:A:636:TRP:CH2	2.49	0.47
1:B:568:MET:HB2	1:B:599:ALA:O	2.14	0.47
1:A:585:PRO:HB3	1:B:544:VAL:HG11	1.97	0.47
1:A:489:HIS:CG	1:A:490:HIS:N	2.82	0.47
1:A:531:ARG:HH21	1:A:638:SER:C	2.17	0.47
1:A:572:LEU:CD2	1:A:596:LEU:HG	2.45	0.47
1:A:584:ASN:HD21	1:A:586:ILE:HD12	1.80	0.47
1:A:543:VAL:HB	1:A:596:LEU:HB3	1.97	0.47
1:B:590:SER:O	2:B:51:HOH:O	2.20	0.47
1:B:633:PRO:HA	1:B:636:TRP:CD1	2.50	0.46
1:B:568:MET:HE2	1:B:600:ASN:OD1	2.16	0.46
1:A:509:PRO:HA	1:A:530:ALA:HB2	1.97	0.46
1:A:514:PRO:HB3	1:A:528:HIS:CE1	2.51	0.45
1:B:556:ARG:HG2	1:B:579:GLU:HG2	2.00	0.44
1:B:531:ARG:HG2	1:B:639:LEU:HB2	1.99	0.44
1:B:632:PRO:HG2	1:B:635:THR:HG23	1.99	0.44
1:A:552:PRO:HG3	1:B:514:PRO:HD3	2.00	0.43
1:B:495:LEU:CD2	1:B:496:SER:O	2.66	0.43
1:B:588:HIS:HD2	1:B:589:PRO:O	2.02	0.42
1:B:608:LEU:C	1:B:608:LEU:HD23	2.39	0.42
1:B:584:ASN:HA	1:B:585:PRO:HD2	1.88	0.42
1:A:635:THR:O	1:A:636:TRP:C	2.58	0.42
1:A:518:TYR:CZ	1:A:520:GLN:HB2	2.55	0.42
1:A:572:LEU:CD2	1:A:596:LEU:CG	2.98	0.41
1:B:604:GLU:HB3	2:B:142:HOH:O	2.19	0.41
1:A:572:LEU:HD21	1:A:596:LEU:HD11	2.01	0.41
1:B:531:ARG:NE	1:B:639:LEU:H	2.19	0.41
1:A:490:HIS:O	1:A:494:GLU:HB2	2.21	0.41
1:A:520:GLN:HB3	1:A:521:HIS:CD2	2.56	0.41
1:B:537:ARG:CG	1:B:538:SER:N	2.82	0.41
1:B:532:ASP:HA	1:B:533:PRO:HD2	1.82	0.40
1:B:568:MET:CE	1:B:600:ASN:OD1	2.70	0.40
1:B:564:VAL:HG22	1:B:565:PRO:CD	2.45	0.40
1:A:635:THR:O	1:A:637:GLY:N	2.55	0.40
1:A:545:VAL:O	1:A:593:THR:HA	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:HOH:O	2:B:142:HOH:O[6_765]	1.27	0.93
1:B:611:LYS:NZ	2:A:103:HOH:O[3_665]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	149/154 (97%)	141 (95%)	7 (5%)	1 (1%)	26 31
1	B	143/154 (93%)	140 (98%)	3 (2%)	0	100 100
All	All	292/308 (95%)	281 (96%)	10 (3%)	1 (0%)	46 57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	566	LYS

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	138/141 (98%)	126 (91%)	12 (9%)	13 15
1	B	132/141 (94%)	126 (96%)	6 (4%)	34 46
All	All	270/282 (96%)	252 (93%)	18 (7%)	20 26

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	508	LYS
1	A	510	SER
1	A	513	LEU
1	A	524	ARG
1	A	564	VAL
1	A	566	LYS
1	A	568	MET
1	A	584	ASN
1	A	596	LEU
1	A	616	MET
1	A	626	ASP
1	A	629	GLN
1	B	495	LEU
1	B	538	SER
1	B	564	VAL
1	B	567	VAL
1	B	571	LYS
1	B	611	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	489	HIS
1	A	521	HIS
1	A	584	ASN
1	A	588	HIS
1	A	619	GLN
1	B	528	HIS
1	B	588	HIS

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 95^{th} 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	151/154 (98%)	0.43	9 (5%)	25	33	17, 23, 35, 53	0
1	B	145/154 (94%)	0.35	14 (9%)	10	14	15, 22, 41, 53	0
All	All	296/308 (96%)	0.39	23 (7%)	16	22	15, 23, 39, 53	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	490	HIS	9.3
1	A	489	HIS	8.0
1	B	538	SER	5.3
1	B	499	SER	4.9
1	A	602	GLN	4.3
1	B	498	ALA	3.9
1	B	495	LEU	3.5
1	A	601	PRO	3.4
1	B	534	LEU	3.3
1	B	537	ARG	3.3
1	B	635	THR	3.2
1	B	535	PRO	3.0
1	A	491	HIS	2.9
1	A	618	ASP	2.9
1	B	601	PRO	2.7
1	A	538	SER	2.6
1	B	536	GLY	2.6
1	B	496	SER	2.3
1	B	513	LEU	2.3
1	B	578	MET	2.1
1	A	567	VAL	2.1
1	B	633	PRO	2.0
1	A	605	LYS	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)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.