



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:02 am GMT

PDB ID : 1OVA
Title : CRYSTAL STRUCTURE OF UNCLEAVED OVALBUMIN AT 1.95
ANGSTROMS RESOLUTION
Authors : Stein, P.E.; Leslie, A.G.W.
Deposited on : 1990-11-26
Resolution : 1.95 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

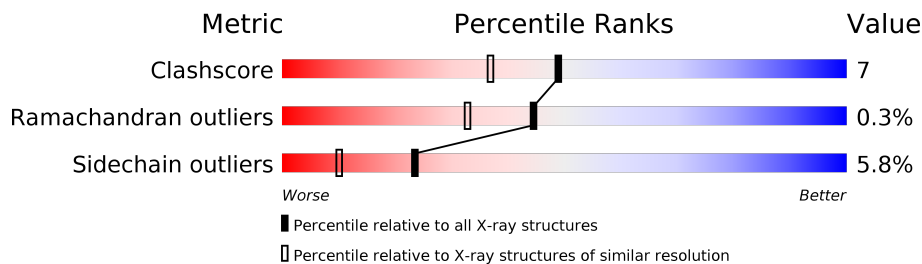
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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))
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	386	
2	B	386	
3	C	386	
3	D	386	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12269 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 OVALBUMIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	P	S	0	0	0
			2940	1876	489	551	2	22			

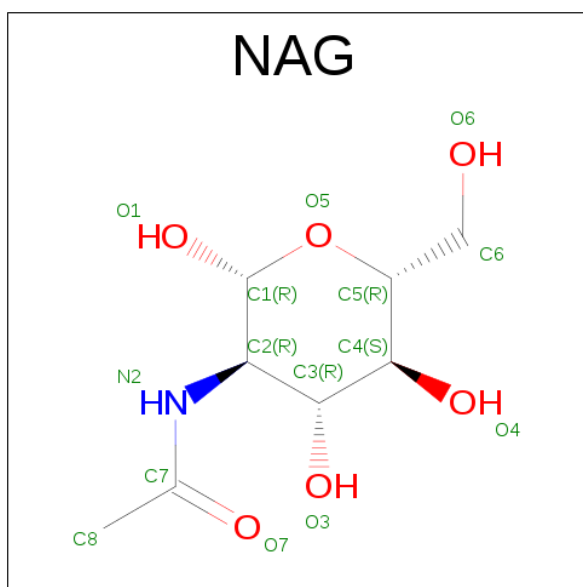
- Molecule 2 is a protein called OVALBUMIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	373	Total	C	N	O	P	S	0	0	0
			2816	1808	454	532	1	21			

- Molecule 3 is a protein called OVALBUMIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	374	Total	C	N	O	S	0	0	0
			2854	1832	469	531	22			
3	D	386	Total	C	N	O	S	0	0	0
			2924	1870	473	559	22			

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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is water.

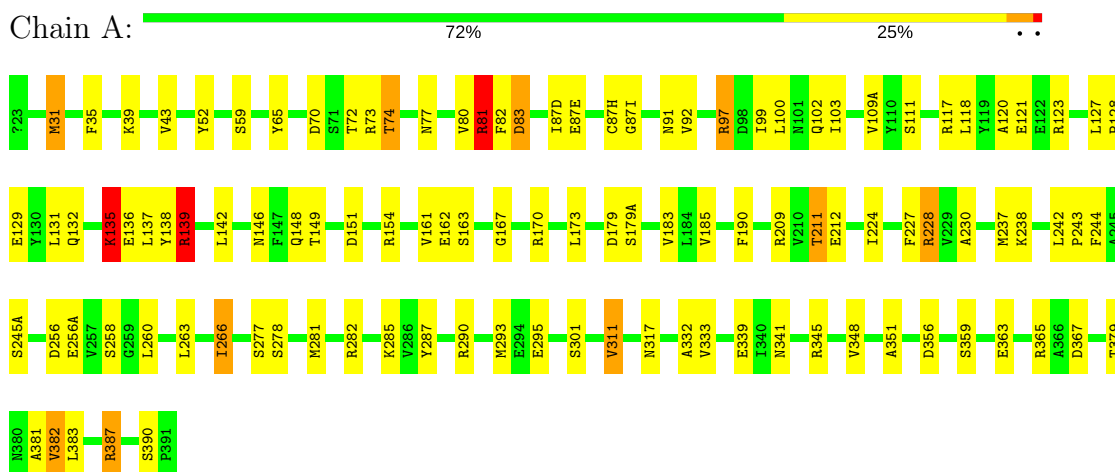
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	167	Total	O	0	0
			167	167		
6	B	156	Total	O	0	0
			156	156		
6	C	172	Total	O	0	0
			172	172		
6	D	183	Total	O	0	0
			183	183		

3 Residue-property plots [i](#)

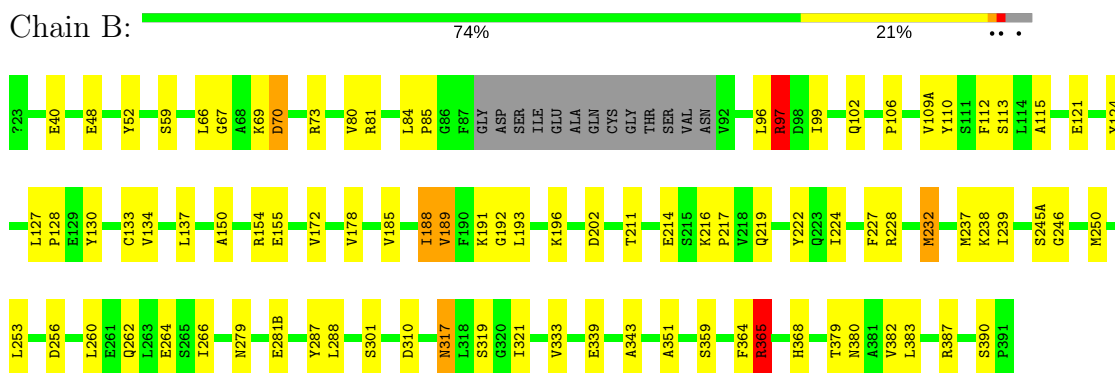
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

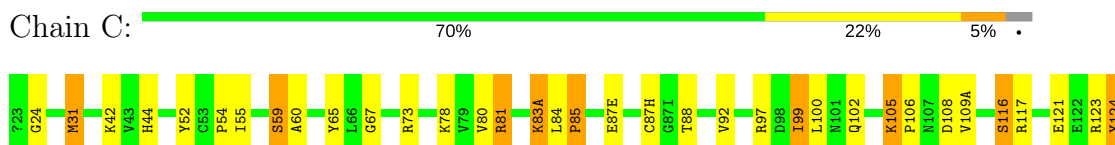
• Molecule 1: OVALBUMIN

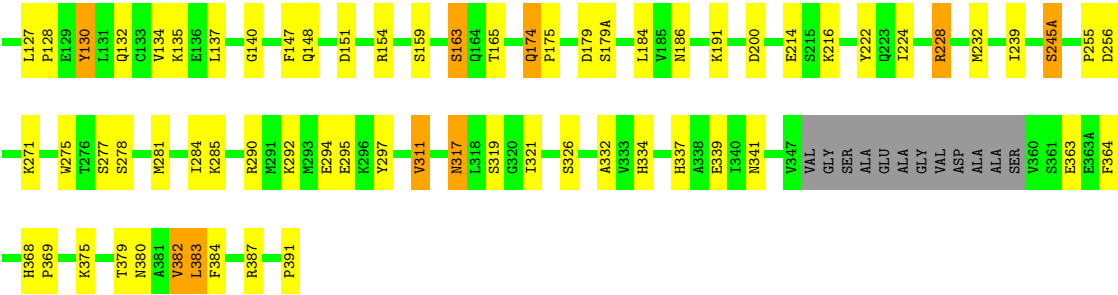


• Molecule 2: OVALBUMIN



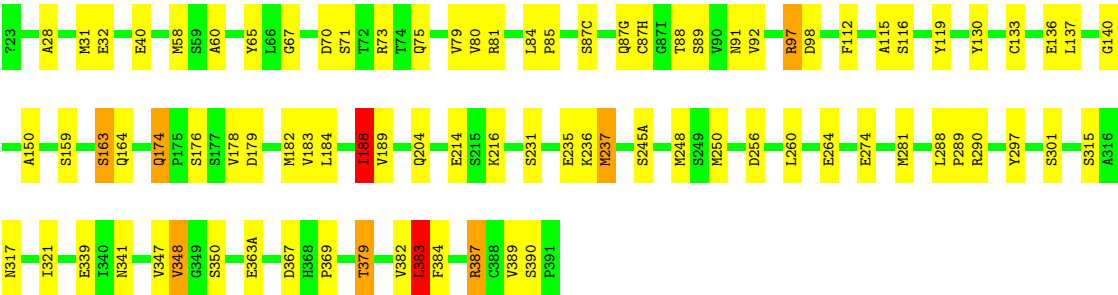
• Molecule 3: OVALBUMIN





● Molecule 3: OVALBUMIN

Chain D: 78% 20% ●●



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.90Å 84.70Å 71.50Å 87.50° 104.00° 108.50°	Depositor
Resolution (Å)	(Not available) – 1.95	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.95)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.169 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12269	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

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, ACE, SEP

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	1.10	2/2972 (0.1%)	1.87	58/4016 (1.4%)
2	B	1.11	2/2858 (0.1%)	1.67	34/3869 (0.9%)
3	C	1.16	2/2907 (0.1%)	1.77	47/3927 (1.2%)
3	D	1.13	2/2978 (0.1%)	1.69	40/4031 (1.0%)
All	All	1.13	8/11715 (0.1%)	1.75	179/15843 (1.1%)

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
3	C	0	1
All	All	0	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	264	GLU	CD-OE1	-7.08	1.17	1.25
2	B	192	GLY	N-CA	6.97	1.56	1.46
1	A	228	ARG	CD-NE	-6.20	1.35	1.46
3	D	159	SER	CA-CB	5.71	1.61	1.52
3	D	264	GLU	CD-OE1	-5.33	1.19	1.25

The worst 5 of 179 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	ARG	CD-NE-CZ	22.24	154.73	123.60
1	A	282	ARG	NE-CZ-NH2	16.65	128.62	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ARG	CD-NE-CZ	15.52	145.33	123.60
2	B	365	ARG	CD-NE-CZ	15.52	145.33	123.60
1	A	345	ARG	NE-CZ-NH1	15.16	127.88	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	87(I)	GLY	Peptide
3	C	245(A)	SER	Peptide

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	2940	0	2906	49	0
2	B	2816	0	2751	38	0
3	C	2854	0	2812	43	0
3	D	2924	0	2865	30	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	12	0	0
4	D	14	0	13	0	0
5	A	1	0	0	0	0
6	A	167	0	0	8	0
6	B	156	0	0	6	0
6	C	172	0	0	0	0
6	D	183	0	0	4	0
All	All	12269	0	11385	157	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 7.

The worst 5 of 157 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)
3:C:174:GLN:HE21	3:C:174:GLN:H	1.13	0.97
1:A:139:ARG:HB3	1:A:139:ARG:HH11	1.46	0.81
1:A:230:ALA:HB2	1:A:281:MET:HG2	1.67	0.76
2:B:239:ILE:HD12	2:B:253:LEU:HG	1.68	0.75
3:C:109(A):VAL:HG21	3:C:245(A):SER:HB2	1.67	0.75

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	382/386 (99%)	358 (94%)	22 (6%)	2 (0%)	32	19
2	B	368/386 (95%)	349 (95%)	18 (5%)	1 (0%)	44	33
3	C	370/386 (96%)	356 (96%)	12 (3%)	2 (0%)	32	19
3	D	384/386 (100%)	369 (96%)	15 (4%)	0	100	100
All	All	1504/1544 (97%)	1432 (95%)	67 (4%)	5 (0%)	44	33

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	ASP
2	B	246	GLY
3	C	88	THR
1	A	43	VAL
3	C	85	PRO

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	308/329 (94%)	289 (94%)	19 (6%)	21	8
2	B	293/330 (89%)	276 (94%)	17 (6%)	23	10
3	C	300/331 (91%)	280 (93%)	20 (7%)	19	7
3	D	310/331 (94%)	296 (96%)	14 (4%)	32	17
All	All	1211/1321 (92%)	1141 (94%)	70 (6%)	23	10

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	359	SER
3	C	137	LEU
3	D	317	ASN
2	B	365	ARG
2	B	390	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	164	GLN
3	C	317	ASN
3	D	317	ASN
3	C	174	GLN
3	C	341	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	SEP	A	350	1	9,9,10	1.37	2 (22%)	9,12,14	2.47	4 (44%)
1	SEP	A	87(C)	1	9,9,10	1.54	2 (22%)	9,12,14	2.90	4 (44%)
2	SEP	B	350	2	9,9,10	1.53	1 (11%)	9,12,14	2.49	4 (44%)

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
1	SEP	A	350	1	-	0/5/8/10	0/0/0/0
1	SEP	A	87(C)	1	-	0/5/8/10	0/0/0/0
2	SEP	B	350	2	-	0/5/8/10	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	350	SEP	P-OG	-2.22	1.53	1.60
1	A	87(C)	SEP	P-OG	-2.07	1.53	1.60
1	A	350	SEP	CA-C	2.62	1.53	1.50
2	B	350	SEP	CA-C	3.11	1.54	1.50
1	A	87(C)	SEP	CA-C	3.15	1.54	1.50

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	350	SEP	OG-P-O1P	-3.09	97.80	106.47
1	A	350	SEP	OG-P-O1P	-2.98	98.11	106.47
1	A	87(C)	SEP	OG-P-O1P	-2.08	100.65	106.47
1	A	87(C)	SEP	OG-CB-CA	2.38	110.51	108.17
1	A	350	SEP	O2P-P-OG	2.46	113.28	106.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	393	1	14,14,15	1.76	4 (28%)	15,19,21	1.96	3 (20%)
4	NAG	B	393	2	14,14,15	1.54	3 (21%)	15,19,21	2.17	5 (33%)
4	NAG	C	393	3	14,14,15	1.47	3 (21%)	15,19,21	1.66	4 (26%)
4	NAG	D	393	3	14,14,15	1.30	1 (7%)	15,19,21	1.53	3 (20%)

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	393	1	-	0/6/23/26	0/1/1/1
4	NAG	B	393	2	-	0/6/23/26	0/1/1/1
4	NAG	C	393	3	-	0/6/23/26	0/1/1/1
4	NAG	D	393	3	-	0/6/23/26	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	393	NAG	O7-C7	-4.15	1.13	1.23
4	B	393	NAG	O7-C7	-3.92	1.14	1.23
4	D	393	NAG	O7-C7	-3.36	1.15	1.23
4	C	393	NAG	O7-C7	-2.82	1.16	1.23
4	A	393	NAG	O5-C5	-2.55	1.38	1.43

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	393	NAG	C1-O5-C5	-5.10	105.14	112.17
4	A	393	NAG	C2-N2-C7	-4.47	116.42	122.94
4	B	393	NAG	C4-C3-C2	-3.21	106.32	111.02
4	B	393	NAG	O3-C3-C2	-3.15	102.64	109.39
4	C	393	NAG	C1-C2-N2	-3.08	105.23	110.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.