



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:46 AM GMT

PDB ID : 2BF1
Title : STRUCTURE OF AN UNLIGANDED AND FULLY-GLYCOSYLATED SIV
GP120 ENVELOPE GLYCOPROTEIN
Authors : Chen, B.; Vogan, E.M.; Gong, H.; Skehel, J.J.; Wiley, D.C.; Harrison, S.C.
Deposited on : 2004-12-02
Resolution : 4.00 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 (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

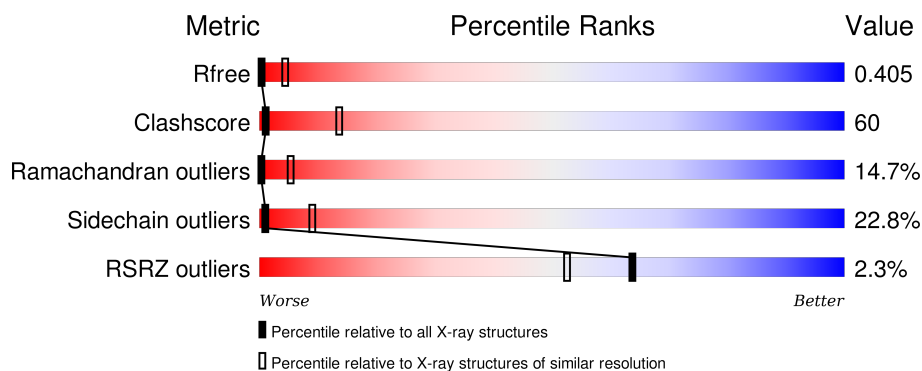
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

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	316	

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
3	FUC	A	1505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NDG	A	1524	X	-	-	-
3	FUC	A	1527	X	-	-	-
4	FUC	A	1511	X	-	-	-
4	NAG	A	1540	X	-	-	-
4	FUC	A	1545	X	-	-	-
5	FUC	A	1514	X	-	-	-
5	FUC	A	1517	X	-	-	-
6	FUC	A	1521	X	-	-	-
7	NDG	A	1522	X	-	-	-
8	NAG	A	1528	X	-	-	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 3086 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 EXTERIOR MEMBRANE GLYCOPROTEIN GP120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	0
			2471	1556	436	456	23			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	4	Total	C	N	O	0	0
			49	28	2	19		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 4 is a polymer of unknown type called SUGAR (6-MER).

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

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			38	22	2	14		
5	A	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	4	Total	C	N	O	0	0
			49	28	2	19		

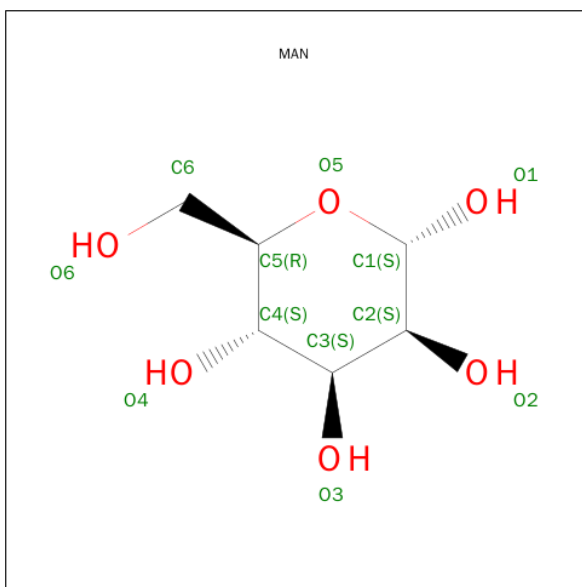
- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 8 is a polymer of unknown type called SUGAR (6-MER).

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

- Molecule 9 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 10 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	5	Total	C	N	O	0	0
			61	34	2	25		

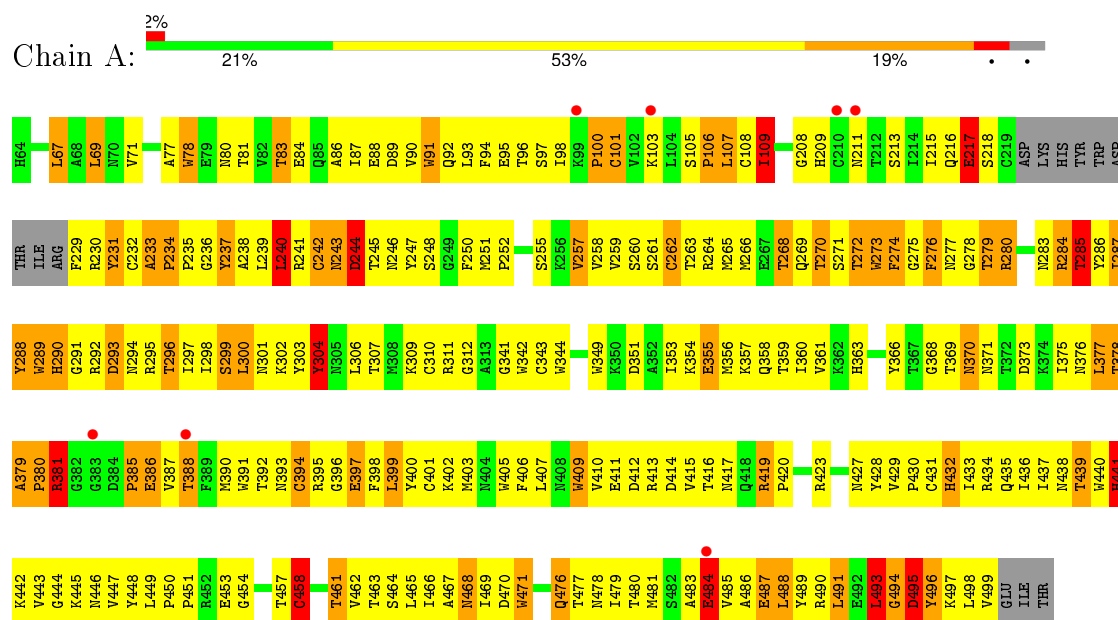
- Molecule 11 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	4	Total	C	N	O	0	0
			50	28	2	20		

3 Residue-property plots

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: EXTERIOR MEMBRANE GLYCOPROTEIN GP120



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	108.05Å 108.05Å 117.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.00 – 4.00 25.58 – 3.99	Depositor EDS
% Data completeness (in resolution range)	98.0 (26.00-4.00) 98.0 (25.58-3.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.97Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.385 , 0.388 0.389 , 0.405	Depositor DCC
R_{free} test set	280 reflections (4.79%)	DCC
Wilson B-factor (Å ²)	175.1	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.03 , 68.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 6186 reflections	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	3086	wwPDB-VP
Average B, all atoms (Å ²)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: FUC, BMA, NAG, NDG, 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	0.67	0/2535	0.92	7/3441 (0.2%)

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
3	A	3	0
4	A	3	0
5	A	2	0
6	A	1	0
7	A	1	0
8	A	1	0
All	All	11	0

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	495	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	244	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	240	LEU	CA-CB-CG	5.67	128.34	115.30
1	A	414	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	293	ASP	CB-CG-OD2	5.29	123.06	118.30

5 of 11 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1505	FUC	C1

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Mol	Chain	Res	Type	Atom
4	A	1511	FUC	C1
5	A	1514	FUC	C1
5	A	1517	FUC	C1
6	A	1521	FUC	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	2471	0	2350	346	0
2	A	28	0	26	0	0
3	A	98	0	86	1	2
4	A	142	0	122	5	0
5	A	76	0	68	8	0
6	A	49	0	43	0	0
7	A	28	0	25	1	0
8	A	72	0	60	8	0
9	A	11	0	10	0	0
10	A	61	0	52	0	0
11	A	50	0	43	1	0
All	All	3086	0	2885	356	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 60.

The worst 5 of 356 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:87:ILE:O	1:A:90:VAL:HG22	1.35	1.25
1:A:92:GLN:NE2	1:A:106:PRO:HG3	1.50	1.24
1:A:88:GLU:HA	1:A:91:TRP:CZ2	1.79	1.16
1:A:285:THR:HG23	1:A:302:LYS:HB2	1.23	1.15
1:A:498:LEU:O	1:A:499:VAL:HG23	1.44	1.14

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1505:FUC:O3	3:A:1505:FUC:O3[8_555]	0.65	1.55
3:A:1505:FUC:C3	3:A:1505:FUC:O3[8_555]	1.92	0.28

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	300/316 (95%)	191 (64%)	65 (22%)	44 (15%)	0 5

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	100	PRO
1	A	107	LEU
1	A	217	GLU
1	A	233	ALA

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	272/284 (96%)	210 (77%)	62 (23%)	1 9

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	299	SER
1	A	370	ASN
1	A	487	GLU
1	A	355	GLU
1	A	381	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	417	ASN
1	A	468	ASN
1	A	441	HIS
1	A	408	ASN
1	A	446	ASN

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 ⓘ

47 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	$\# Z > 2$
3	NDG	A	1502	1,3	14,14,15	0.70	0	15,19,21	0.84	0
3	NAG	A	1503	3	14,14,15	0.87	1 (7%)	15,19,21	1.07	1 (6%)
3	BMA	A	1504	3	11,11,12	0.79	0	14,15,17	1.18	0
3	FUC	A	1505	3	10,10,11	0.76	0	14,14,16	1.64	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1506	1,4	14,14,15	0.75	0	15,19,21	1.56	4 (26%)
4	NAG	A	1507	4	14,14,15	1.03	1 (7%)	15,19,21	1.74	2 (13%)
4	BMA	A	1508	4	11,11,12	0.97	1 (9%)	14,15,17	2.03	3 (21%)
4	MAN	A	1509	4	11,11,12	0.54	0	14,15,17	1.58	1 (7%)
4	MAN	A	1510	4	11,11,12	0.58	0	14,15,17	1.57	3 (21%)
4	FUC	A	1511	4	10,10,11	0.74	0	14,14,16	1.20	1 (7%)
5	NDG	A	1512	1,5	14,14,15	0.65	0	15,19,21	1.77	4 (26%)
5	NAG	A	1513	5	14,14,15	0.69	0	15,19,21	1.51	2 (13%)
5	FUC	A	1514	5	10,10,11	0.74	0	14,14,16	1.22	1 (7%)
5	NDG	A	1515	1,5	14,14,15	0.50	0	15,19,21	1.68	3 (20%)
5	NAG	A	1516	5	14,14,15	0.53	0	15,19,21	1.47	2 (13%)
5	FUC	A	1517	5	10,10,11	0.58	0	14,14,16	1.06	1 (7%)
6	NAG	A	1518	1,6	14,14,15	0.66	0	15,19,21	1.81	4 (26%)
6	NAG	A	1519	6	14,14,15	0.61	0	15,19,21	1.19	1 (6%)
6	BMA	A	1520	6	11,11,12	0.54	0	14,15,17	1.08	1 (7%)
6	FUC	A	1521	6	10,10,11	0.59	0	14,14,16	1.35	2 (14%)
7	NDG	A	1522	1,7	14,14,15	0.63	0	15,19,21	1.65	3 (20%)
7	NAG	A	1523	7	14,14,15	0.75	0	15,19,21	0.98	1 (6%)
3	NDG	A	1524	1,3	14,14,15	0.69	0	15,19,21	1.31	2 (13%)
3	NAG	A	1525	3	14,14,15	0.74	0	15,19,21	1.64	2 (13%)
3	BMA	A	1526	3	11,11,12	0.89	1 (9%)	14,15,17	1.65	2 (14%)
3	FUC	A	1527	3	10,10,11	0.69	0	14,14,16	1.54	2 (14%)
8	NAG	A	1528	1,8	14,14,15	0.79	1 (7%)	15,19,21	1.23	1 (6%)
8	NAG	A	1529	8	14,14,15	0.43	0	15,19,21	3.18	3 (20%)
8	BMA	A	1530	8	11,11,12	0.98	0	14,15,17	2.04	5 (35%)
8	MAN	A	1531	8	11,11,12	0.51	0	14,15,17	2.03	2 (14%)
8	MAN	A	1532	9,8	11,11,12	0.66	0	14,15,17	1.08	2 (14%)
8	MAN	A	1534	8	11,11,12	0.57	0	14,15,17	1.93	3 (21%)
10	NAG	A	1535	1,10	14,14,15	0.55	0	15,19,21	1.28	1 (6%)
10	NAG	A	1536	10	14,14,15	1.00	1 (7%)	15,19,21	1.78	5 (33%)
10	BMA	A	1537	10	11,11,12	0.73	0	14,15,17	1.26	2 (14%)
10	MAN	A	1538	10	11,11,12	0.83	0	14,15,17	2.00	1 (7%)
10	MAN	A	1539	10	11,11,12	0.57	0	14,15,17	1.28	1 (7%)
4	NAG	A	1540	1,4	14,14,15	0.82	1 (7%)	15,19,21	1.84	3 (20%)
4	NAG	A	1541	4	14,14,15	0.62	0	15,19,21	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BMA	A	1542	4	11,11,12	0.56	0	14,15,17	3.05	3 (21%)
4	MAN	A	1543	4	11,11,12	0.54	0	14,15,17	1.74	2 (14%)
4	MAN	A	1544	4	11,11,12	0.72	0	14,15,17	0.99	1 (7%)
4	FUC	A	1545	4	10,10,11	1.07	0	14,14,16	1.73	2 (14%)
11	NDG	A	1546	1,11	14,14,15	0.57	0	15,19,21	2.02	3 (20%)
11	NAG	A	1547	11	14,14,15	0.60	0	15,19,21	1.38	2 (13%)
11	BMA	A	1548	11	11,11,12	0.73	0	14,15,17	1.24	2 (14%)
11	MAN	A	1549	11	11,11,12	0.58	0	14,15,17	1.59	2 (14%)

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	NDG	A	1502	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1503	3	-	0/6/23/26	0/1/1/1
3	BMA	A	1504	3	-	0/2/19/22	0/1/1/1
3	FUC	A	1505	3	1/1/4/5	0/0/17/20	0/1/1/1
4	NAG	A	1506	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1507	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1508	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1509	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1510	4	-	0/2/19/22	0/1/1/1
4	FUC	A	1511	4	1/1/4/5	0/0/17/20	0/1/1/1
5	NDG	A	1512	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1513	5	-	0/6/23/26	0/1/1/1
5	FUC	A	1514	5	1/1/4/5	0/0/17/20	0/1/1/1
5	NDG	A	1515	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1516	5	-	0/6/23/26	0/1/1/1
5	FUC	A	1517	5	1/1/4/5	0/0/17/20	0/1/1/1
6	NAG	A	1518	1,6	-	1/6/23/26	0/1/1/1
6	NAG	A	1519	6	-	0/6/23/26	0/1/1/1
6	BMA	A	1520	6	-	0/2/19/22	0/1/1/1
6	FUC	A	1521	6	1/1/4/5	0/0/17/20	0/1/1/1
7	NDG	A	1522	1,7	1/1/5/7	1/6/23/26	0/1/1/1
7	NAG	A	1523	7	-	0/6/23/26	0/1/1/1
3	NDG	A	1524	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	1525	3	-	0/6/23/26	0/1/1/1
3	BMA	A	1526	3	-	0/2/19/22	0/1/1/1
3	FUC	A	1527	3	1/1/4/5	0/0/17/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	1528	1,8	1/1/5/7	0/6/23/26	0/1/1/1
8	NAG	A	1529	8	-	0/6/23/26	0/1/1/1
8	BMA	A	1530	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1531	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1532	9,8	-	0/2/19/22	0/1/1/1
8	MAN	A	1534	8	-	0/2/19/22	0/1/1/1
10	NAG	A	1535	1,10	-	0/6/23/26	0/1/1/1
10	NAG	A	1536	10	-	0/6/23/26	0/1/1/1
10	BMA	A	1537	10	-	0/2/19/22	0/1/1/1
10	MAN	A	1538	10	-	0/2/19/22	0/1/1/1
10	MAN	A	1539	10	-	0/2/19/22	0/1/1/1
4	NAG	A	1540	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	1541	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1542	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1543	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1544	4	-	0/2/19/22	0/1/1/1
4	FUC	A	1545	4	1/1/4/5	0/0/17/20	0/1/1/1
11	NDG	A	1546	1,11	-	0/6/23/26	0/1/1/1
11	NAG	A	1547	11	-	0/6/23/26	0/1/1/1
11	BMA	A	1548	11	-	0/2/19/22	0/1/1/1
11	MAN	A	1549	11	-	0/2/19/22	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1503	NAG	C1-C2	2.20	1.55	1.52
8	A	1528	NAG	C1-C2	2.27	1.55	1.52
4	A	1508	BMA	C2-C3	2.37	1.55	1.52
3	A	1526	BMA	C2-C3	2.50	1.55	1.52
4	A	1507	NAG	C1-C2	2.51	1.55	1.52

The worst 5 of 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1529	NAG	C4-C3-C2	-8.80	97.55	111.23
4	A	1545	FUC	O2-C2-C3	-4.37	101.33	110.12
5	A	1515	NDG	C3-C4-C5	-4.12	103.02	110.20
5	A	1512	NDG	C4-C3-C2	-3.95	105.09	111.23
8	A	1528	NAG	C2-N2-C7	-3.81	118.15	123.04

5 of 11 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	1522	NDG	C1
4	A	1540	NAG	C1
5	A	1517	FUC	C1
8	A	1528	NAG	C1
4	A	1545	FUC	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1518	NAG	O7-C7-N2-C2
7	A	1522	NDG	O7-C7-N2-C2

There are no ring outliers.

17 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1503	NAG	1	0
3	A	1504	BMA	1	0
3	A	1505	FUC	0	2
4	A	1506	NAG	1	0
4	A	1508	BMA	1	0
4	A	1510	MAN	1	0
5	A	1512	NDG	3	0
5	A	1513	NAG	2	0
5	A	1514	FUC	2	0
5	A	1515	NDG	4	0
5	A	1517	FUC	2	0
7	A	1522	NDG	1	0
8	A	1528	NAG	3	0
8	A	1529	NAG	6	0
4	A	1540	NAG	3	0
4	A	1545	FUC	2	0
11	A	1546	NDG	1	0

5.6 Ligand geometry

3 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	$\# Z > 2$
2	NAG	A	1500	1	14,14,15	0.66	0	15,19,21	1.35	1 (6%)
2	NAG	A	1501	1	14,14,15	0.90	1 (7%)	15,19,21	0.97	0
9	MAN	A	1533	8	11,11,12	0.66	0	14,15,17	1.81	4 (28%)

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	1500	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1501	1	-	0/6/23/26	0/1/1/1
9	MAN	A	1533	8	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1501	NAG	O6-C6	2.43	1.52	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	NAG	C2-N2-C7	-3.87	118.07	123.04
9	A	1533	MAN	O5-C1-C2	-2.74	106.41	110.86
9	A	1533	MAN	O4-C4-C3	-2.32	105.11	110.34
9	A	1533	MAN	C1-O5-C5	3.35	116.49	112.25
9	A	1533	MAN	C3-C4-C5	3.69	116.63	110.20

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 ⓘ

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 [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	304/316 (96%)	-0.09	7 (2%) 64 52	96, 124, 157, 183	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	99	LYS	3.0
1	A	484	GLU	2.7
1	A	388	THR	2.7
1	A	210	CYS	2.6
1	A	103	LYS	2.3

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
8	MAN	A	1534	11/12	0.76	0.33	-0.28	123,129,133,136	0
3	NDG	A	1524	14/15	0.82	0.25	-0.71	136,140,147,148	0
11	NDG	A	1546	14/15	0.85	0.20	-0.90	123,131,138,141	0
8	NAG	A	1529	14/15	0.79	0.28	-1.21	118,125,134,134	0
4	NAG	A	1540	14/15	0.88	0.18	-1.51	105,108,110,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
10	MAN	A	1538	11/12	0.81	0.18	-	195,203,214,216	0
3	BMA	A	1526	11/12	0.50	0.73	-	165,174,183,185	0
7	NDG	A	1522	14/15	0.83	0.20	-	182,192,205,210	0
5	FUC	A	1517	10/11	0.74	0.29	-	154,158,162,163	0
8	BMA	A	1530	11/12	0.77	0.28	-	129,133,140,141	0
4	MAN	A	1510	11/12	0.87	0.16	-	132,137,143,145	0
3	NDG	A	1502	14/15	0.88	0.21	-	110,113,117,117	0
8	NAG	A	1528	14/15	0.72	0.56	-	114,122,128,131	0
7	NAG	A	1523	14/15	0.90	0.15	-	185,198,212,214	0
3	NAG	A	1525	14/15	0.50	0.37	-	151,156,162,163	0
10	MAN	A	1539	11/12	0.78	0.23	-	164,169,173,173	0
4	FUC	A	1545	10/11	0.85	0.24	-	112,117,121,122	0
5	NDG	A	1515	14/15	0.79	0.18	-	137,146,154,159	0
4	FUC	A	1511	10/11	0.92	0.13	-	109,111,113,114	0
3	BMA	A	1504	11/12	0.88	0.19	-	132,135,141,141	0
5	NDG	A	1512	14/15	0.83	0.21	-	122,125,128,129	0
11	NAG	A	1547	14/15	0.86	0.20	-	145,149,157,158	0
4	NAG	A	1506	14/15	0.76	0.28	-	101,106,109,110	0
4	NAG	A	1507	14/15	0.66	0.63	-	112,115,119,123	0
4	MAN	A	1543	11/12	0.90	0.14	-	117,119,124,126	0
4	MAN	A	1509	11/12	0.93	0.09	-	136,140,144,147	0
11	BMA	A	1548	11/12	0.87	0.28	-	163,171,177,180	0
5	NAG	A	1513	14/15	0.81	0.34	-	133,138,145,146	0
8	MAN	A	1531	11/12	0.72	0.34	-	143,149,156,158	0
4	BMA	A	1542	11/12	0.89	0.21	-	111,114,117,118	0
5	NAG	A	1516	14/15	0.92	0.13	-	162,170,178,178	0
3	NAG	A	1503	14/15	0.78	0.27	-	114,121,126,130	0
11	MAN	A	1549	11/12	0.76	0.26	-	176,184,190,194	0
4	NAG	A	1541	14/15	0.88	0.21	-	107,110,112,112	0
10	NAG	A	1535	14/15	0.90	0.21	-	159,163,167,168	0
8	MAN	A	1532	11/12	0.81	0.49	-	140,146,153,155	0
10	BMA	A	1537	11/12	0.76	0.36	-	177,185,195,199	0
10	NAG	A	1536	14/15	0.55	0.57	-	168,172,184,186	0
6	FUC	A	1521	10/11	0.85	0.18	-	121,126,130,132	0
5	FUC	A	1514	10/11	0.86	0.21	-	121,127,129,132	0
6	NAG	A	1519	14/15	0.81	0.24	-	125,135,142,145	0
6	NAG	A	1518	14/15	0.87	0.19	-	120,123,128,130	0
4	MAN	A	1544	11/12	0.83	0.21	-	117,121,125,126	0
3	FUC	A	1527	10/11	0.86	0.27	-	136,141,143,145	0
4	BMA	A	1508	11/12	0.84	0.14	-	125,129,136,136	0
3	FUC	A	1505	10/11	0.83	0.41	-	114,117,121,121	0
6	BMA	A	1520	11/12	0.92	0.10	-	149,153,162,164	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(Å ²)	Q<0.9
2	NAG	A	1501	14/15	0.82	0.31	-	140,145,150,155	0
9	MAN	A	1533	11/12	0.83	0.20	-	160,163,168,170	0
2	NAG	A	1500	14/15	0.91	0.19	-	147,151,157,160	0

6.5 Other polymers [i](#)

There are no such residues in this entry.