



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:02 PM UTC

PDB ID : 3IDY / pdb\_00003idy  
Title : Crystal structure of HIV-gp120 core in complex with CD4-binding site antibody b13, space group C2221  
Authors : Chen, L.; Kwon, Y.D.; Zhou, T.; Wu, X.; O'Dell, S.; Cavacini, L.; Hessel, A.J.; Pancera, M.; Tang, M.; Xu, L.; Yang, Z.Y.; Zhang, M.Y.; Arthos, J.; Burton, D.R.; Dimitrov, D.S.; Nabel, G.J.; Posner, M.; Sodroski, J.; Wyatt, R.; Mascola, J.R.; Kwong, P.D.  
Deposited on : 2009-07-22  
Resolution : 3.20 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](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

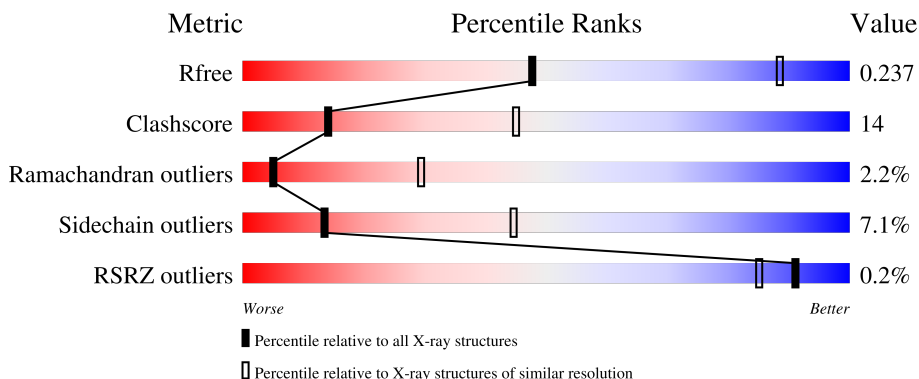
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
$R_{free}$	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	317	65% 26% . . .
1	G	317	66% 26% . . .
2	B	231	63% 32% . .
2	H	231	65% 32% . .

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Mol	Chain	Length	Quality of chain
3	C	215	 % 72% 23% 5%
3	L	215	 73% 22%

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	NAG	G	588	X	-	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12038 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 HIV-1 HxBc2 gp120 core.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	G	306	Total 2367	C 1483	N 412	O 448	S 24	0	0	0
1	A	303	Total 2354	C 1476	N 409	O 445	S 24	0	0	0

- Molecule 2 is a protein called Fab b13 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	229	Total 1730	C 1092	N 297	O 334	S 7	0	0	0
2	B	229	Total 1730	C 1092	N 297	O 334	S 7	0	0	0

- Molecule 3 is a protein called Fab b13 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	214	Total 1654	C 1028	N 284	O 337	S 5	0	0	0
3	C	214	Total 1654	C 1028	N 284	O 337	S 5	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	O S	0	0
			5	4 1		

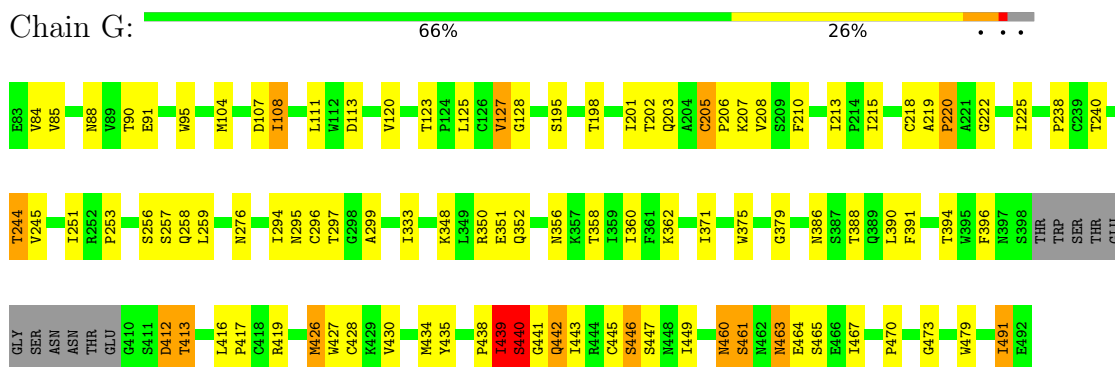
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	30	Total	O	0	0
			30	30		
6	H	12	Total	O	0	0
			12	12		
6	L	12	Total	O	0	0
			12	12		
6	A	41	Total	O	0	0
			41	41		
6	B	30	Total	O	0	0
			30	30		
6	C	27	Total	O	0	0
			27	27		

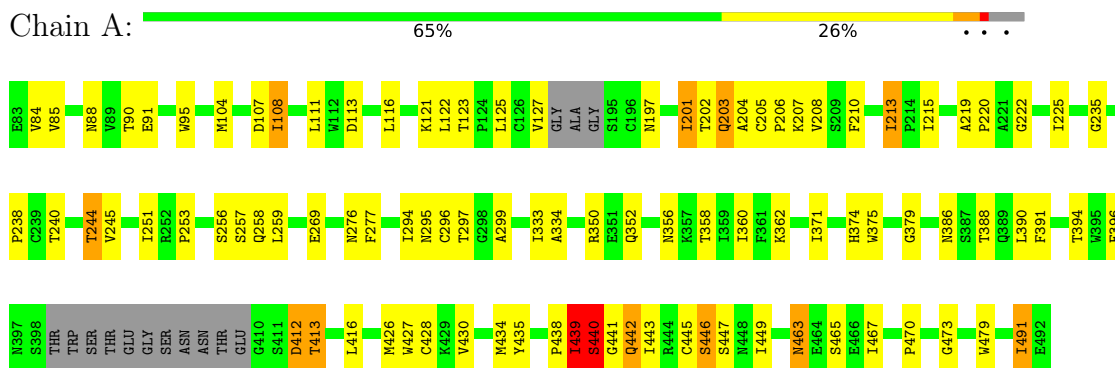
### 3 Residue-property plots [i](#)

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 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.

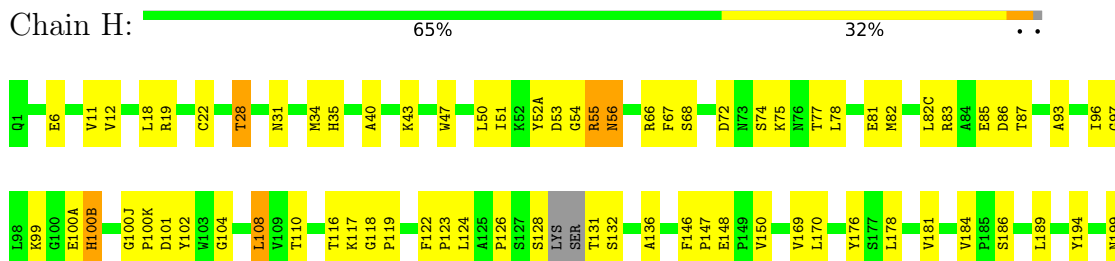
- Molecule 1: HIV-1 HxBc2 gp120 core



- Molecule 1: HIV-1 HxBc2 gp120 core



- Molecule 2: Fab b13 heavy chain





- Molecule 2: Fab b13 heavy chain

Chain B: 63% 32% ..



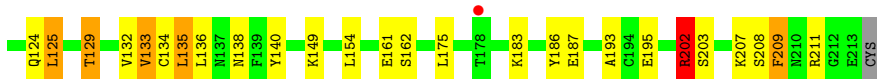
- Molecule 3: Fab b13 light chain

Chain L: 73% 22% .



- Molecule 3: Fab b13 light chain

Chain C: 72% 23% 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.17Å 204.32Å 216.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.20 – 3.20 43.20 – 3.20	Depositor EDS
% Data completeness (in resolution range)	47.1 (43.20-3.20) 90.1 (43.20-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 2.77Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.196 , 0.237 0.192 , 0.237	Depositor DCC
$R_{free}$ test set	1900 reflections (3.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	92.9	Xtrriage
Anisotropy	0.346	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 111.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12038	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	151.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SO4

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	0.34	0/2401	0.76	5/3254 (0.2%)
1	G	0.33	0/2415	0.77	3/3274 (0.1%)
2	B	0.32	1/1771 (0.1%)	0.70	0/2407
2	H	0.39	2/1771 (0.1%)	0.72	2/2407 (0.1%)
3	C	0.29	0/1688	0.75	1/2291 (0.0%)
3	L	0.31	0/1688	0.74	0/2291
All	All	0.33	3/11734 (0.0%)	0.75	11/15924 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	100(B)	HIS	ND1-CE1	5.24	1.37	1.32
2	B	56	ASN	CG-OD1	5.22	1.33	1.23
2	H	56	ASN	CG-OD1	5.02	1.33	1.23

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	441	GLY	N-CA-C	-7.39	106.19	114.40
1	G	441	GLY	N-CA-C	-7.30	106.30	114.40
2	H	100(B)	HIS	CB-CG-CD2	-6.63	122.58	131.20
1	A	439	ILE	N-CA-C	6.42	117.05	110.82
1	G	439	ILE	N-CA-C	6.36	116.99	110.82

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	2354	0	2285	67	0
1	G	2367	0	2298	69	0
2	B	1730	0	1696	72	0
2	H	1730	0	1696	63	0
3	C	1654	0	1602	36	0
3	L	1654	0	1602	41	0
4	A	196	0	181	10	0
4	G	196	0	182	7	0
5	G	5	0	0	1	0
6	A	41	0	0	2	0
6	B	30	0	0	9	0
6	C	27	0	0	3	0
6	G	30	0	0	2	0
6	H	12	0	0	0	0
6	L	12	0	0	0	0
All	All	12038	0	11542	334	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 14.

The worst 5 of 334 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:H:100(A):GLU:HG2	3:L:53:ASN:ND2	1.85	0.92
2:H:100(A):GLU:HG2	3:L:53:ASN:HD21	1.35	0.90
1:G:461:SER:CA	4:G:963:NAG:H82	2.03	0.89
1:G:388:THR:HG21	4:G:886:NAG:H5	1.54	0.88
1:G:463:ASN:HD22	1:G:464:GLU:H	1.30	0.80

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	297/317 (94%)	258 (87%)	32 (11%)	7 (2%)	4	28
1	G	302/317 (95%)	260 (86%)	33 (11%)	9 (3%)	3	23
2	B	225/231 (97%)	183 (81%)	35 (16%)	7 (3%)	3	22
2	H	225/231 (97%)	189 (84%)	32 (14%)	4 (2%)	6	34
3	C	212/215 (99%)	185 (87%)	24 (11%)	3 (1%)	9	39
3	L	212/215 (99%)	183 (86%)	26 (12%)	3 (1%)	9	39
All	All	1473/1526 (96%)	1258 (85%)	182 (12%)	33 (2%)	5	29

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	440	SER
1	A	440	SER
2	B	100(A)	GLU
1	G	379	GLY
2	H	55	ARG

### 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	271/281 (96%)	249 (92%)	22 (8%)	11	39
1	G	271/281 (96%)	247 (91%)	24 (9%)	9	34
2	B	189/191 (99%)	183 (97%)	6 (3%)	34	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	189/191 (99%)	183 (97%)	6 (3%)	34 65
3	C	189/190 (100%)	172 (91%)	17 (9%)	9 34
3	L	189/190 (100%)	172 (91%)	17 (9%)	9 34
All	All	1298/1324 (98%)	1206 (93%)	92 (7%)	13 44

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	244	THR
2	B	116	THR
1	A	356	ASN
1	A	440	SER
3	C	15	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	199	ASN
3	C	138	ASN
2	H	199	ASN
3	L	160	GLN
1	A	229	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry

29 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
4	NAG	G	730	1	14,14,15	0.45	0	17,19,21	0.88	1 (5%)
4	NAG	A	730	1	14,14,15	0.53	0	17,19,21	0.95	1 (5%)
4	NAG	A	734	1	14,14,15	0.46	0	17,19,21	0.91	1 (5%)
4	NAG	G	741	1	14,14,15	0.42	0	17,19,21	0.95	1 (5%)
4	NAG	A	892	1	14,14,15	0.63	0	17,19,21	1.10	1 (5%)
4	NAG	G	588	1	14,14,15	0.53	0	17,19,21	0.83	1 (5%)
4	NAG	A	948	1	14,14,15	0.49	0	17,19,21	1.24	3 (17%)
4	NAG	A	588	1	14,14,15	0.60	0	17,19,21	1.49	2 (11%)
4	NAG	G	839	1	14,14,15	0.55	0	17,19,21	0.98	1 (5%)
4	NAG	A	839	1	14,14,15	0.54	0	17,19,21	1.02	1 (5%)
4	NAG	G	963	1	14,14,15	0.50	0	17,19,21	0.78	1 (5%)
4	NAG	A	776	1	14,14,15	1.26	1 (7%)	17,19,21	1.34	1 (5%)
4	NAG	A	789	1	14,14,15	0.50	0	17,19,21	0.74	0
4	NAG	G	795	1	14,14,15	0.50	0	17,19,21	0.66	0
4	NAG	A	886	1	14,14,15	0.63	0	17,19,21	0.70	0
4	NAG	A	963	1	14,14,15	0.59	0	17,19,21	1.06	2 (11%)
5	SO4	G	1003	-	4,4,4	0.23	0	6,6,6	0.10	0
4	NAG	G	762	1	14,14,15	0.62	0	17,19,21	1.29	2 (11%)
4	NAG	A	795	1	14,14,15	0.53	0	17,19,21	0.78	0
4	NAG	G	789	1	14,14,15	0.45	0	17,19,21	0.84	0
4	NAG	G	856	1	14,14,15	0.57	0	17,19,21	1.40	2 (11%)
4	NAG	G	886	1	14,14,15	0.64	0	17,19,21	1.12	1 (5%)
4	NAG	A	856	1	14,14,15	0.57	0	17,19,21	1.34	2 (11%)
4	NAG	A	762	1	14,14,15	0.53	0	17,19,21	0.98	1 (5%)
4	NAG	G	948	1	14,14,15	0.41	0	17,19,21	2.26	4 (23%)
4	NAG	G	892	1	14,14,15	0.57	0	17,19,21	0.94	1 (5%)
4	NAG	G	734	1	14,14,15	0.61	0	17,19,21	1.00	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	G	776	1	14,14,15	0.46	0	17,19,21	1.00	1 (5%)
4	NAG	A	741	1	14,14,15	0.58	0	17,19,21	0.72	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
4	NAG	G	730	1	-	0/6/23/26	0/1/1/1
4	NAG	A	730	1	-	4/6/23/26	0/1/1/1
4	NAG	A	734	1	-	1/6/23/26	0/1/1/1
4	NAG	G	741	1	-	2/6/23/26	0/1/1/1
4	NAG	A	892	1	-	4/6/23/26	0/1/1/1
4	NAG	G	588	1	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	A	948	1	-	0/6/23/26	0/1/1/1
4	NAG	A	588	1	-	1/6/23/26	0/1/1/1
4	NAG	G	839	1	-	3/6/23/26	0/1/1/1
4	NAG	A	839	1	-	2/6/23/26	0/1/1/1
4	NAG	G	963	1	-	0/6/23/26	0/1/1/1
4	NAG	A	776	1	-	2/6/23/26	0/1/1/1
4	NAG	A	789	1	-	1/6/23/26	0/1/1/1
4	NAG	G	795	1	-	3/6/23/26	0/1/1/1
4	NAG	A	886	1	-	0/6/23/26	0/1/1/1
4	NAG	A	963	1	-	2/6/23/26	0/1/1/1
4	NAG	G	762	1	-	2/6/23/26	0/1/1/1
4	NAG	A	795	1	-	4/6/23/26	0/1/1/1
4	NAG	G	789	1	-	3/6/23/26	0/1/1/1
4	NAG	G	856	1	-	2/6/23/26	0/1/1/1
4	NAG	G	886	1	-	2/6/23/26	0/1/1/1
4	NAG	A	856	1	-	2/6/23/26	0/1/1/1
4	NAG	A	762	1	-	2/6/23/26	0/1/1/1
4	NAG	G	948	1	-	0/6/23/26	0/1/1/1
4	NAG	G	892	1	-	0/6/23/26	0/1/1/1
4	NAG	G	734	1	-	1/6/23/26	0/1/1/1
4	NAG	G	776	1	-	0/6/23/26	0/1/1/1
4	NAG	A	741	1	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	776	NAG	C8-C7	-4.28	1.41	1.50

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	948	NAG	C1-O5-C5	6.99	121.56	112.19
4	A	856	NAG	C1-O5-C5	4.24	117.86	112.19
4	G	948	NAG	C4-C3-C2	-4.13	104.96	111.02
4	A	588	NAG	C2-N2-C7	3.78	127.97	122.90
4	A	776	NAG	C2-N2-C7	-3.75	117.88	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	G	588	NAG	C1

5 of 50 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	588	NAG	C3-C2-N2-C7
4	G	588	NAG	C8-C7-N2-C2
4	G	588	NAG	O7-C7-N2-C2
4	G	741	NAG	C8-C7-N2-C2
4	G	741	NAG	O7-C7-N2-C2

There are no ring outliers.

10 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	734	NAG	1	0
4	A	588	NAG	2	0
4	G	963	NAG	4	0
4	A	789	NAG	2	0
4	A	886	NAG	1	0
5	G	1003	SO4	1	0
4	G	762	NAG	2	0
4	A	795	NAG	3	0
4	G	886	NAG	1	0
4	A	762	NAG	1	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	303/317 (95%)	-0.29	0 <a href="#">100</a> <a href="#">100</a>	95, 125, 199, 271	0
1	G	306/317 (96%)	-0.32	0 <a href="#">100</a> <a href="#">100</a>	92, 125, 205, 271	0
2	B	229/231 (99%)	-0.31	1 (0%) <a href="#">88</a> <a href="#">79</a>	100, 167, 237, 289	0
2	H	229/231 (99%)	-0.17	0 <a href="#">100</a> <a href="#">100</a>	91, 165, 234, 288	0
3	C	214/215 (99%)	-0.21	2 (0%) <a href="#">81</a> <a href="#">64</a>	104, 151, 234, 303	0
3	L	214/215 (99%)	-0.23	0 <a href="#">100</a> <a href="#">100</a>	93, 145, 232, 262	0
All	All	1495/1526 (97%)	-0.26	3 (0%) <a href="#">91</a> <a href="#">85</a>	91, 142, 231, 303	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	178	THR	2.3
3	C	102	THR	2.2
2	B	139	GLY	2.2

### 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 oligosaccharides in this entry.

### 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. The B-factors column lists the minimum,

median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	NAG	A	856	14/15	-0.11	0.17	170,250,287,291	0
4	NAG	G	856	14/15	-0.05	0.13	184,252,279,292	0
4	NAG	A	588	14/15	0.32	0.13	143,206,225,236	0
4	NAG	A	963	14/15	0.41	0.11	170,225,242,246	0
4	NAG	G	730	14/15	0.47	0.09	158,229,236,237	0
4	NAG	A	730	14/15	0.48	0.11	180,212,233,238	0
4	NAG	G	588	14/15	0.52	0.09	187,247,265,266	0
4	NAG	A	741	14/15	0.59	0.12	113,213,241,245	0
4	NAG	G	741	14/15	0.60	0.12	146,204,232,238	0
4	NAG	G	734	14/15	0.70	0.09	158,195,210,225	0
4	NAG	A	776	14/15	0.70	0.09	133,183,194,197	0
5	SO4	G	1003	5/5	0.73	0.09	162,173,190,220	0
4	NAG	A	734	14/15	0.74	0.10	165,188,209,216	0
4	NAG	A	892	14/15	0.74	0.11	132,192,205,212	0
4	NAG	A	839	14/15	0.75	0.10	131,213,220,222	0
4	NAG	G	776	14/15	0.81	0.08	151,175,183,195	0
4	NAG	G	892	14/15	0.83	0.08	118,177,197,209	0
4	NAG	G	839	14/15	0.84	0.10	153,188,211,216	0
4	NAG	G	795	14/15	0.85	0.10	124,161,166,195	0
4	NAG	G	963	14/15	0.85	0.07	211,229,239,241	0
4	NAG	A	795	14/15	0.86	0.09	120,152,170,189	0
4	NAG	A	789	14/15	0.86	0.09	112,128,141,152	0
4	NAG	G	948	14/15	0.87	0.08	86,148,198,201	0
4	NAG	A	948	14/15	0.88	0.08	117,140,165,165	0
4	NAG	G	789	14/15	0.89	0.10	108,146,178,179	0
4	NAG	A	886	14/15	0.92	0.10	113,154,172,179	0
4	NAG	G	886	14/15	0.94	0.08	109,142,159,171	0
4	NAG	G	762	14/15	0.96	0.07	76,96,128,130	0
4	NAG	A	762	14/15	0.96	0.08	77,94,125,144	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.