



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:07 am GMT

PDB ID : 2VDO  
Title : INTEGRIN ALPHAIIIBETA3 HEADPIECE BOUND TO FIBRINOGEN  
GAMMA CHAIN PEPTIDE, HHLGGAKQAGDV  
Authors : Springer, T.A.; Zhu, J.; Xiao, T.  
Deposited on : 2007-10-10  
Resolution : 2.51 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](mailto: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.

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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) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

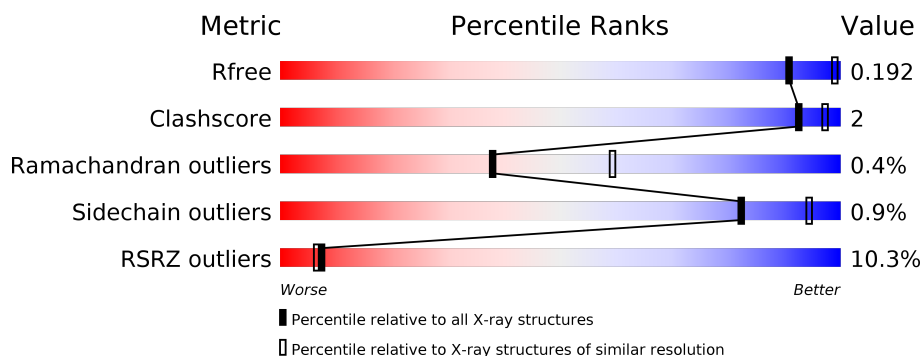
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.51 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))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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  $\geq 3$ , 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	452	<div> <div>8%</div> <div>96%</div> <div>.</div> </div>
2	B	461	<div> <div>20%</div> <div>92%</div> <div>6%</div> <div>.</div> </div>
3	C	12	<div> <div>25%</div> <div>83%</div> <div>17%</div> </div>
4	H	221	<div> <div>2%</div> <div>95%</div> <div>.</div> <div>.</div> </div>
5	L	214	<div> <div>2%</div> <div>95%</div> <div>5%</div> </div>

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
10	MAN	B	3323	X	-	-	-
10	MAN	B	3324	X	-	-	-
11	MAN	B	3373	X	-	-	-
11	MAN	B	3374	-	-	-	X
11	MAN	B	3376	X	-	-	-
11	MAN	B	3377	X	-	-	-
6	GOL	B	1462	-	-	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 11786 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 INTEGRIN ALPHA-IIB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	9	0
			3528	2240	615	665	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	282	GLY	ALA	CONFLICT SEE REMARK 9	UNP P08514

- Molecule 2 is a protein called INTEGRIN BETA-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	455	Total	C	N	O	S	0	12	0
			3577	2235	606	703	33			

- Molecule 3 is a protein called FIBRINOGEN, GAMMA POLYPEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	12	Total	C	N	O	0	0	0
			84	50	18	16			

- Molecule 4 is a protein called MONOCLONAL ANTIBODY 10E5 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	219	Total	C	N	O	S	0	3	0
			1678	1064	270	338	6			

- Molecule 5 is a protein called MONOCLONAL ANTIBODY 10E5 LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	214	Total	C	N	O	S	0	7	0
			1671	1042	272	346	11			

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Ca	0	0
			2	2		
7	A	4	Total	Ca	0	0
			4	4		

- Molecule 8 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Mg	0	0
			1	1		

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

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

- Molecule 11 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	7	Total	C	N	O	0	0
			83	46	2	35		

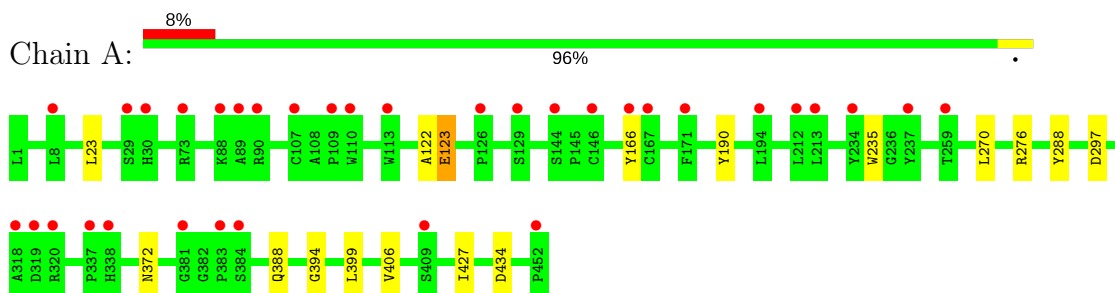
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	393	Total 393	O 393	0	0
12	B	208	Total 208	O 208	0	0
12	C	14	Total 14	O 14	0	0
12	H	205	Total 205	O 205	0	0
12	L	223	Total 223	O 223	0	0

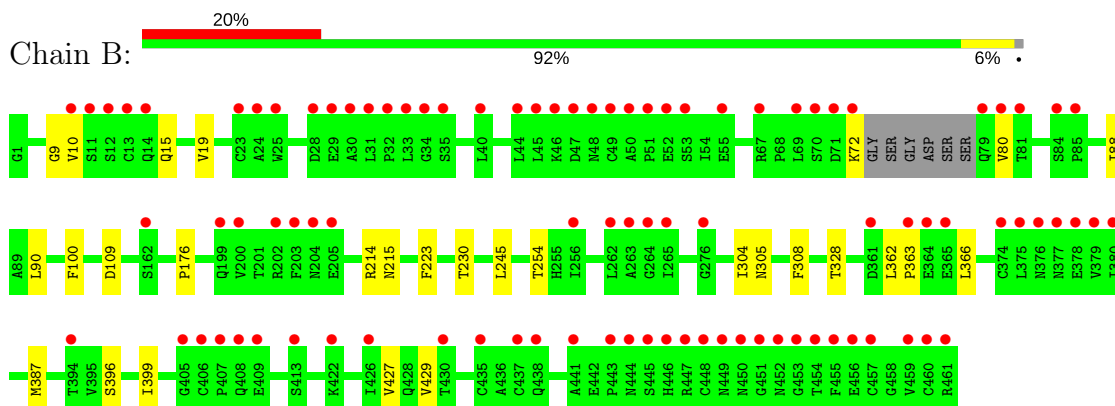
### 3 Residue-property plots [i](#)

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.

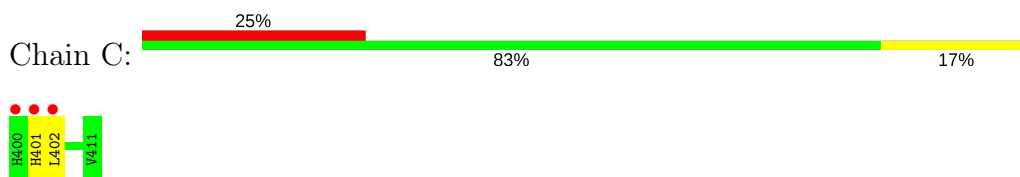
#### • Molecule 1: INTEGRIN ALPHA-IIB



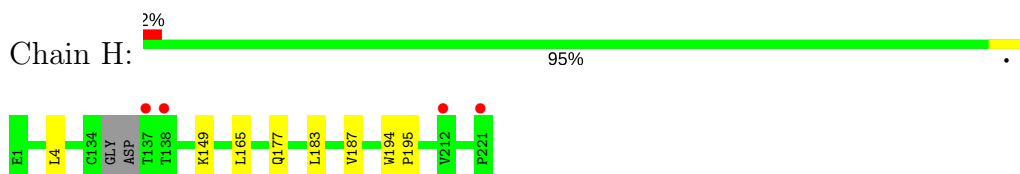
#### • Molecule 2: INTEGRIN BETA-3



#### • Molecule 3: FIBRINOGEN, GAMMA POLYPEPTIDE



#### • Molecule 4: MONOCLONAL ANTIBODY 10E5 HEAVY CHAIN





- Molecule 5: MONOCLONAL ANTIBODY 10E5 LIGHT CHAIN

Chain L:  2% 95% 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	148.33Å 148.33Å 176.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.13 – 2.51 46.10 – 2.51	Depositor EDS
% Data completeness (in resolution range)	97.3 (46.13-2.51) 97.0 (46.10-2.51)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.83 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, $R_{free}$	0.148 , 0.190 0.152 , 0.192	Depositor DCC
$R_{free}$ test set	3805 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.2	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 46.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11786	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage'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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, CA, NAG, 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	0.35	0/3640	0.55	0/4957
2	B	0.33	0/3661	0.49	0/4960
3	C	0.41	0/85	0.56	0/111
4	H	0.33	0/1730	0.52	0/2369
5	L	0.36	0/1733	0.55	0/2349
All	All	0.34	0/10849	0.53	0/14746

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
10	B	2	0
11	B	3	0
All	All	5	0

There are no bond length outliers.

There are no bond angle outliers.

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	B	3323	MAN	C1
10	B	3324	MAN	C1
11	B	3373	MAN	C1
11	B	3376	MAN	C1
11	B	3377	MAN	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	3528	0	3374	10	0
2	B	3577	0	3512	13	0
3	C	84	0	77	0	0
4	H	1678	0	1637	9	0
5	L	1671	0	1599	12	0
6	A	6	0	8	0	0
6	B	6	0	7	0	0
7	A	4	0	0	0	0
7	B	2	0	0	0	0
8	A	28	0	26	0	0
8	B	14	0	13	0	0
9	B	1	0	0	0	0
10	B	61	0	52	0	0
11	B	83	0	70	0	0
12	A	393	0	0	0	0
12	B	208	0	0	0	0
12	C	14	0	0	0	0
12	H	205	0	0	0	0
12	L	223	0	0	1	0
All	All	11786	0	10375	39	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 2.

All (39) 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)
4:H:177[B]:GLN:OE1	5:L:160[B]:LEU:HD11	1.09	1.23
4:H:177[B]:GLN:OE1	5:L:160[B]:LEU:CD1	1.97	1.12
2:B:88[B]:ILE:HD11	2:B:427:VAL:HG22	1.78	0.66
1:A:235:TRP:CZ2	1:A:270:LEU:HD11	2.33	0.64
4:H:177[B]:GLN:CD	5:L:160[B]:LEU:HD21	2.21	0.60
5:L:136:LEU:HD12	5:L:136:LEU:N	2.21	0.54
4:H:177[B]:GLN:OE1	5:L:160[B]:LEU:CG	2.55	0.54
2:B:230:THR:HG23	2:B:304:ILE:HD12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:308:PHE:CE2	2:B:328:THR:HG21	2.44	0.53
5:L:48:ILE:HD13	5:L:54:LEU:HD12	1.91	0.53
1:A:235:TRP:HZ2	1:A:270:LEU:HD11	1.72	0.53
2:B:399:ILE:N	2:B:399:ILE:HD12	2.25	0.52
5:L:48:ILE:CD1	5:L:54:LEU:HD12	2.40	0.51
5:L:105[B]:GLU:HG3	5:L:173:TYR:OH	2.11	0.51
1:A:394:GLY:HA2	1:A:399:LEU:HD23	1.92	0.50
2:B:245:LEU:HD23	2:B:305:ASN:HB2	1.92	0.50
4:H:165:LEU:CD2	4:H:187:VAL:HG21	2.41	0.49
1:A:270:LEU:HD23	1:A:276[A]:ARG:HA	1.95	0.49
1:A:122:ALA:O	1:A:123:GLU:HB2	2.12	0.48
5:L:122:SER:O	5:L:126:THR:HG23	2.13	0.48
1:A:270:LEU:HD23	1:A:276[B]:ARG:HA	1.95	0.48
2:B:90:LEU:HD11	2:B:100:PHE:CE2	2.50	0.47
4:H:165:LEU:HD21	4:H:187:VAL:HG21	1.97	0.46
5:L:45:MET:HE3	12:L:4065:HOH:O	2.15	0.45
2:B:366:LEU:HD11	2:B:429:VAL:HG21	1.99	0.45
2:B:223:PHE:CZ	2:B:254:THR:HG21	2.53	0.43
1:A:122:ALA:O	1:A:123:GLU:CB	2.67	0.42
1:A:388:GLN:NE2	1:A:406:VAL:HG11	2.34	0.42
2:B:72:LYS:NZ	2:B:109:ASP:OD1	2.52	0.42
1:A:427:ILE:HG22	1:A:434:ASP:OD1	2.20	0.42
4:H:177[B]:GLN:NE2	5:L:160[B]:LEU:HD21	2.34	0.42
2:B:15:GLN:O	2:B:19:VAL:HG23	2.20	0.41
2:B:176:PRO:HB2	2:B:214:ARG:HB3	2.03	0.41
4:H:4:LEU:N	4:H:4:LEU:HD12	2.35	0.41
2:B:88[B]:ILE:CD1	2:B:427:VAL:HG22	2.49	0.41
4:H:194:TRP:CG	4:H:195:PRO:HA	2.55	0.41
2:B:362:LEU:HD12	2:B:363:PRO:HD2	2.03	0.40
5:L:4:MET:HE2	5:L:90:GLN:HB3	2.03	0.40
1:A:297:ASP:O	1:A:372:ASN:HB2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	458/452 (101%)	446 (97%)	11 (2%)	1 (0%)	51	73
2	B	460/461 (100%)	438 (95%)	19 (4%)	3 (1%)	25	43
3	C	10/12 (83%)	6 (60%)	3 (30%)	1 (10%)	1	0
4	H	218/221 (99%)	214 (98%)	4 (2%)	0	100	100
5	L	220/214 (103%)	215 (98%)	5 (2%)	0	100	100
All	All	1366/1360 (100%)	1319 (97%)	42 (3%)	5 (0%)	38	59

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
2	B	9[A]	GLY
2	B	80	VAL
3	C	402	LEU
2	B	10	VAL

### 5.3.2 Protein sidechains ⓘ

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	368/360 (102%)	364 (99%)	4 (1%)	78	92
2	B	414/409 (101%)	410 (99%)	4 (1%)	80	93
3	C	7/7 (100%)	6 (86%)	1 (14%)	4	7
4	H	192/190 (101%)	190 (99%)	2 (1%)	80	93
5	L	196/188 (104%)	196 (100%)	0	100	100
All	All	1177/1154 (102%)	1166 (99%)	11 (1%)	82	94

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	166	TYR
1	A	190	TYR
1	A	288	TYR
2	B	215	ASN
2	B	387[A]	MET
2	B	387[B]	MET
2	B	396	SER
3	C	401	HIS
4	H	149	LYS
4	H	183	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	388	GLN
2	B	316	ASN
2	B	342	GLN
2	B	428	GLN

### 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 ⓘ

12 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
10	NAG	B	3320	10,2	14,14,15	0.59	0	15,19,21	0.91	1 (6%)
10	NAG	B	3321	10	14,14,15	0.68	0	15,19,21	1.03	1 (6%)
10	MAN	B	3322	10	11,11,12	0.73	0	13,15,17	1.98	3 (23%)
10	MAN	B	3323	10	11,11,12	0.67	0	13,15,17	0.85	1 (7%)
10	MAN	B	3324	10	11,11,12	0.60	0	13,15,17	0.96	1 (7%)
11	NAG	B	3371	11,2	14,14,15	0.64	0	15,19,21	0.98	1 (6%)
11	NAG	B	3372	11	14,14,15	0.52	0	15,19,21	0.75	0
11	MAN	B	3373	11	11,11,12	0.63	0	13,15,17	0.84	0
11	MAN	B	3374	-	11,11,12	0.62	0	13,15,17	0.71	0
11	MAN	B	3375	11	11,11,12	0.60	0	13,15,17	1.94	3 (23%)
11	MAN	B	3376	11	11,11,12	0.57	0	13,15,17	0.81	0
11	MAN	B	3377	11	11,11,12	0.70	0	13,15,17	1.40	3 (23%)

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
10	NAG	B	3320	10,2	-	0/6/23/26	0/1/1/1
10	NAG	B	3321	10	-	0/6/23/26	0/1/1/1
10	MAN	B	3322	10	-	0/2/19/22	0/1/1/1
10	MAN	B	3323	10	1/1/4/5	0/2/19/22	0/1/1/1
10	MAN	B	3324	10	1/1/4/5	0/2/19/22	0/1/1/1
11	NAG	B	3371	11,2	-	0/6/23/26	0/1/1/1
11	NAG	B	3372	11	-	0/6/23/26	0/1/1/1
11	MAN	B	3373	11	1/1/4/5	0/2/19/22	0/1/1/1
11	MAN	B	3374	-	-	0/2/19/22	0/1/1/1
11	MAN	B	3375	11	-	0/2/19/22	0/1/1/1
11	MAN	B	3376	11	1/1/4/5	0/2/19/22	0/1/1/1
11	MAN	B	3377	11	1/1/4/5	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	3377	MAN	O5-C1-C2	-2.76	106.46	110.79
11	B	3371	NAG	O5-C1-C2	-2.52	107.97	111.47
10	B	3320	NAG	O5-C1-C2	-2.44	108.08	111.47
10	B	3323	MAN	O5-C1-C2	-2.26	107.25	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	3324	MAN	O5-C1-C2	-2.22	107.32	110.79
11	B	3375	MAN	C2-C3-C4	-2.21	107.02	110.88
11	B	3377	MAN	C1-C2-C3	-2.19	106.88	109.65
10	B	3321	NAG	C4-C3-C2	2.26	114.33	111.02
10	B	3322	MAN	C2-C3-C4	2.34	114.95	110.88
11	B	3375	MAN	C1-O5-C5	2.53	115.66	112.17
11	B	3377	MAN	C3-C4-C5	2.91	115.34	110.22
10	B	3322	MAN	C1-O5-C5	4.04	117.73	112.17
10	B	3322	MAN	C1-C2-C3	4.38	115.20	109.65
11	B	3375	MAN	O3-C3-C2	5.39	119.83	110.02

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	B	3323	MAN	C1
11	B	3376	MAN	C1
11	B	3373	MAN	C1
11	B	3377	MAN	C1
10	B	3324	MAN	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 7 are monoatomic - leaving 5 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	$\# Z  > 2$
6	GOL	A	1453	-	5,5,5	0.46	0	5,5,5	0.07	0
8	NAG	A	3015	-	14,14,15	0.46	0	15,19,21	0.64	0
8	NAG	A	3249	-	14,14,15	0.49	0	15,19,21	0.63	0
6	GOL	B	1462	7	5,5,5	0.41	0	5,5,5	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	B	3099	2	14,14,15	0.42	0	15,19,21	1.12	1 (6%)

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
6	GOL	A	1453	-	-	0/4/4/4	0/0/0/0
8	NAG	A	3015	-	-	0/6/23/26	0/1/1/1
8	NAG	A	3249	-	-	0/6/23/26	0/1/1/1
6	GOL	B	1462	7	-	0/4/4/4	0/0/0/0
8	NAG	B	3099	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	3099	NAG	O5-C1-C2	-3.13	107.11	111.47

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

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	452/452 (100%)	0.60	34 (7%) 15 15	46, 58, 76, 102	1 (0%)
2	B	455/461 (98%)	1.18	94 (20%) 1 1	45, 68, 102, 113	2 (0%)
3	C	12/12 (100%)	0.89	3 (25%) 1 0	48, 69, 133, 141	0
4	H	219/221 (99%)	0.22	4 (1%) 69 70	42, 60, 81, 119	1 (0%)
5	L	214/214 (100%)	0.23	4 (1%) 67 69	42, 58, 72, 109	1 (0%)
All	All	1352/1360 (99%)	0.68	139 (10%) 7 6	42, 60, 96, 141	5 (0%)

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	453	GLY	10.3
2	B	448	CYS	10.1
2	B	451	GLY	9.2
5	L	214	CYS	9.0
2	B	454	THR	8.8
2	B	444	ASN	7.7
2	B	452	ASN	7.6
2	B	11	SER	7.4
2	B	460	CYS	7.2
4	H	137	THR	7.1
2	B	405	GLY	7.1
2	B	34	GLY	6.5
2	B	443	PRO	6.2
2	B	408	GLN	6.2
2	B	33	LEU	6.2
2	B	447	ARG	6.0
2	B	461	ARG	5.7
2	B	376	ASN	5.7
2	B	450	ASN	5.6
2	B	378	GLU	5.6

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Mol	Chain	Res	Type	RSRZ
2	B	32	PRO	5.3
2	B	455	PHE	5.3
2	B	48	ASN	5.3
2	B	379	VAL	5.2
2	B	459	VAL	5.1
2	B	30	ALA	5.1
1	A	337[A]	PRO	5.0
2	B	422	LYS	5.0
2	B	406	CYS	4.6
2	B	446	HIS	4.6
2	B	445	SER	4.4
2	B	81	THR	4.4
1	A	320	ARG	4.4
4	H	138	THR	4.4
3	C	400	HIS	4.3
2	B	70	SER	4.1
1	A	452	PRO	4.1
2	B	35	SER	4.0
2	B	79	GLN	4.0
2	B	409	GLU	4.0
2	B	31	LEU	4.0
2	B	28	ASP	4.0
2	B	437	CYS	3.9
2	B	377	ASN	3.9
2	B	49	CYS	3.8
2	B	364	GLU	3.8
2	B	24	ALA	3.7
2	B	456	GLU	3.7
2	B	374	CYS	3.7
2	B	14	GLN	3.6
5	L	213	GLU	3.5
1	A	318	ALA	3.5
1	A	90[A]	ARG	3.4
2	B	85	PRO	3.4
2	B	426	ILE	3.4
2	B	449	ASN	3.3
2	B	29	GLU	3.3
1	A	110	TRP	3.3
3	C	401	HIS	3.2
2	B	47	ASP	3.1
1	A	381	GLY	3.1
2	B	204	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	319	ASP	3.1
2	B	84	SER	3.0
2	B	375	LEU	3.0
2	B	199	GLN	3.0
4	H	221	PRO	3.0
2	B	69	LEU	2.9
2	B	80	VAL	2.9
5	L	202	THR	2.9
2	B	25	TRP	2.8
1	A	234	TYR	2.8
2	B	394	THR	2.8
2	B	380	ILE	2.8
1	A	144	SER	2.7
5	L	201	SER	2.7
2	B	71	ASP	2.7
2	B	10	VAL	2.7
2	B	262	LEU	2.7
1	A	113	TRP	2.7
1	A	29	SER	2.7
2	B	67	ARG	2.7
2	B	407	PRO	2.7
3	C	402	LEU	2.6
2	B	46	LYS	2.6
2	B	413	SER	2.6
2	B	162	SER	2.6
2	B	12	SER	2.6
2	B	51	PRO	2.6
2	B	203	PHE	2.6
2	B	53	SER	2.6
2	B	263	ALA	2.5
2	B	72	LYS	2.5
1	A	171	PHE	2.5
2	B	265	ILE	2.5
2	B	44	LEU	2.5
2	B	361	ASP	2.5
2	B	45	LEU	2.4
1	A	384	SER	2.4
2	B	13	CYS	2.4
2	B	256	ILE	2.4
2	B	441	ALA	2.4
4	H	212	VAL	2.4
1	A	30	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	212	LEU	2.4
2	B	200	VAL	2.4
1	A	107	CYS	2.4
2	B	435	CYS	2.4
1	A	126	PRO	2.4
1	A	166	TYR	2.3
2	B	202	ARG	2.3
1	A	8	LEU	2.3
2	B	365	GLU	2.3
2	B	438	GLN	2.3
1	A	129	SER	2.3
2	B	23	CYS	2.3
2	B	205	GLU	2.3
1	A	194	LEU	2.3
1	A	73	ARG	2.2
1	A	89	ALA	2.2
1	A	88	LYS	2.2
2	B	430	THR	2.2
2	B	52	GLU	2.2
2	B	457	CYS	2.2
1	A	109	PRO	2.2
1	A	383	PRO	2.2
2	B	276	GLY	2.2
1	A	167	CYS	2.2
1	A	259	THR	2.1
1	A	146	CYS	2.1
1	A	237	TYR	2.1
2	B	40	LEU	2.1
1	A	213	LEU	2.1
2	B	264	GLY	2.1
1	A	338	HIS	2.1
2	B	363	PRO	2.0
1	A	409	SER	2.0
2	B	55	GLU	2.0
2	B	50	ALA	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
11	MAN	B	3374	11/12	0.89	0.25	2.00	92,96,97,98	11
11	NAG	B	3371	14/15	0.91	0.24	0.29	81,86,88,90	0
11	MAN	B	3375	11/12	0.93	0.31	-	79,85,91,96	0
10	NAG	B	3320	14/15	0.96	0.14	-	53,62,70,78	0
10	MAN	B	3322	11/12	0.79	0.42	-	117,124,127,131	0
11	MAN	B	3376	11/12	0.79	0.18	-	78,79,81,82	0
11	MAN	B	3373	11/12	0.87	0.33	-	89,96,98,98	0
11	MAN	B	3377	11/12	0.80	0.33	-	100,101,103,103	0
10	MAN	B	3324	11/12	0.68	0.43	-	131,133,135,136	0
10	NAG	B	3321	14/15	0.91	0.28	-	83,89,99,109	0
10	MAN	B	3323	11/12	0.72	0.32	-	126,128,129,129	0
11	NAG	B	3372	14/15	0.87	0.27	-	78,91,96,98	0

### 6.4 Ligands ⓘ

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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	GOL	B	1462	6/6	0.91	0.27	4.99	72,72,73,74	0
6	GOL	A	1453	6/6	0.89	0.25	-0.89	65,72,76,79	0
7	CA	A	2004	1/1	0.97	0.07	-2.11	67,67,67,67	0
7	CA	A	2007	1/1	0.97	0.10	-2.76	65,65,65,65	0
7	CA	A	2005	1/1	0.93	0.08	-3.09	61,61,61,61	0
7	CA	B	2002	1/1	0.99	0.06	-3.87	50,50,50,50	0
7	CA	A	2006	1/1	0.94	0.05	-4.56	70,70,70,70	0
9	MG	B	2001	1/1	0.97	0.04	-4.96	30,30,30,30	0
7	CA	B	2003	1/1	0.99	0.03	-8.36	41,41,41,41	0
8	NAG	A	3015	14/15	0.53	0.51	-	93,97,99,99	14
8	NAG	A	3249	14/15	0.60	0.50	-	102,103,104,105	14
8	NAG	B	3099	14/15	0.77	0.53	-	105,112,117,118	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.