



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:59 PM GMT

PDB ID : 2VDP  
Title : INTEGRIN ALPHAIIIBBETA3 HEADPIECE BOUND TO FIBRINOGEN  
GAMMA CHAIN PEPTIDE,LGGAKQAGDV  
Authors : Springer, T.A.; Zhu, J.; Xiao, T.  
Deposited on : 2007-10-10  
Resolution : 2.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

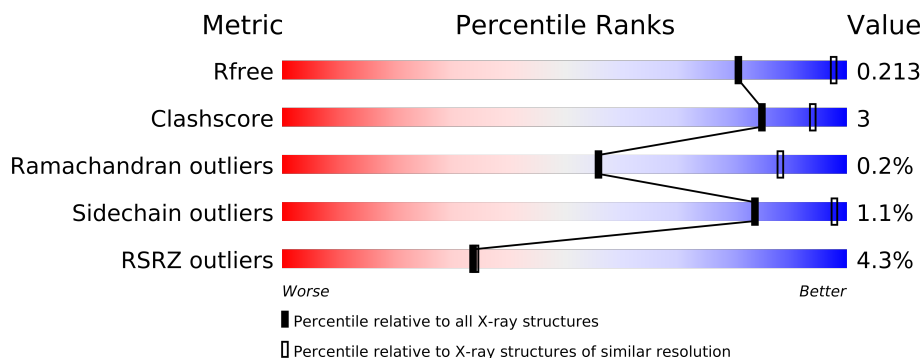
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.80 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))
$R_{free}$	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	452	
2	B	461	
3	C	10	
4	H	221	
5	L	214	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
6	GOL	A	1453	-	X
6	GOL	B	1462	-	X
8	NAG	B	3099	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 11208 atoms, of which 0 are hydrogen and 0 are deuterium.

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	8	0
			3514	2232	611	663	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	5	0
			3554	2217	606	697	34			

- Molecule 3 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	0	0	0
			52	30	10	12			

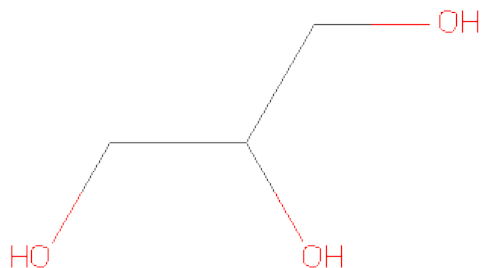
- Molecule 4 is a protein called MONOCLONAL ANTIBODY 10E5 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	219	Total	C	N	O	S	0	2	0
			1672	1060	269	337	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	4	0
			1654	1030	269	346	9			

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

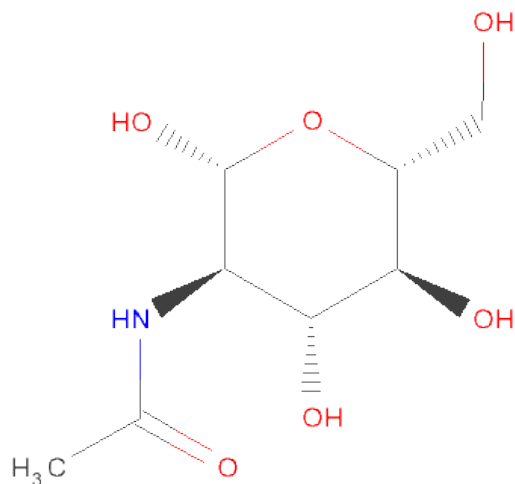


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

- 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.

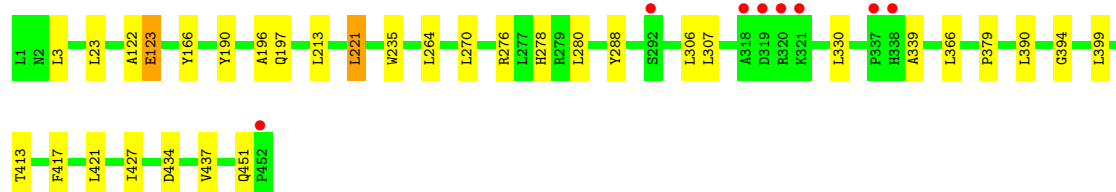
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	228	Total 228	O 228	0	0
12	B	102	Total 102	O 102	0	0
12	C	7	Total 7	O 7	0	0
12	H	106	Total 106	O 106	0	0
12	L	114	Total 114	O 114	0	0

### 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.

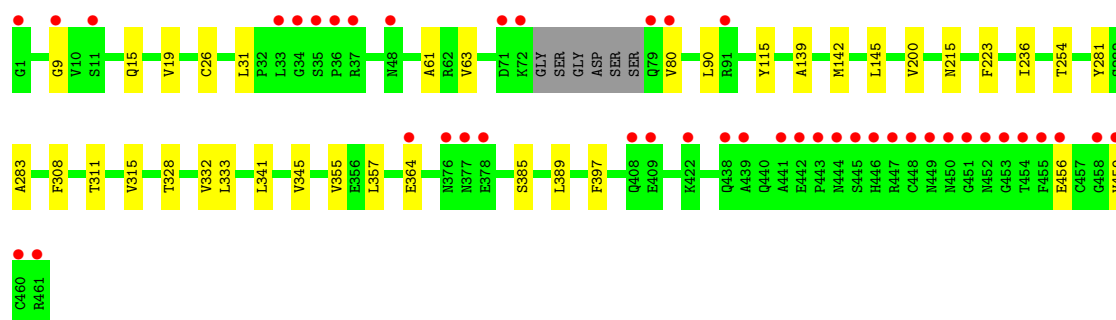
#### • Molecule 1: INTEGRIN ALPHA-IIB

Chain A: 



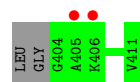
#### • Molecule 2: INTEGRIN BETA-3

Chain B: 



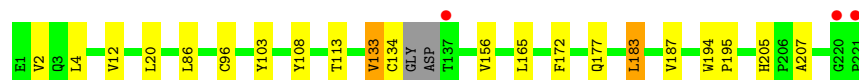
#### • Molecule 3: FIBRINOGEN

Chain C: 



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

Chain H: 



#### • Molecule 5: MONOCLONAL ANTIBODY 10E5 LIGHT CHAIN

Chain L: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	148.43Å 148.43Å 177.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.23 – 2.80 37.52 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.3 (46.23-2.80) 93.6 (37.52-2.80)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.89 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, $R_{free}$	0.156 , 0.204 0.168 , 0.213	Depositor DCC
$R_{free}$ test set	2660 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.8	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 29.4	EDS
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 52252 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11208	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.34	0/3623	0.53	0/4935
2	B	0.33	0/3626	0.49	0/4913
3	C	0.52	0/51	0.56	0/65
4	H	0.32	0/1721	0.50	0/2357
5	L	0.33	0/1702	0.52	0/2308
All	All	0.33	0/10723	0.51	0/14578

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	1	0
11	B	1	0
All	All	2	0

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	B	3322	MAN	C1
11	B	3373	MAN	C1

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3514	0	3356	20	0
2	B	3554	0	3493	18	0
3	C	52	0	49	0	0
4	H	1672	0	1629	16	0
5	L	1654	0	1573	7	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	228	0	0	1	0
12	B	102	0	0	0	0
12	C	7	0	0	0	0
12	H	106	0	0	1	0
12	L	114	0	0	0	0
All	All	11208	0	10276	58	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (58) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:270:LEU:HD23	1:A:276[A]:ARG:HA	1.65	0.78
1:A:270:LEU:HD23	1:A:276[B]:ARG:HA	1.66	0.77
5:L:122:SER:O	5:L:126:THR:HG23	2.01	0.61
1:A:235:TRP:HZ2	1:A:270:LEU:HD11	1.65	0.60
1:A:196:ALA:HA	1:A:221:LEU:HD12	1.84	0.59
4:H:12:VAL:HG21	4:H:86:LEU:HD13	1.88	0.56
1:A:235:TRP:CZ2	1:A:270:LEU:HD11	2.42	0.55
2:B:139:ALA:HB1	2:B:200:VAL:HG13	1.90	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:H:20:LEU:HD22	4:H:113:THR:HG21	1.89	0.53
4:H:205:HIS:CE1	4:H:207:ALA:HB3	2.44	0.53
1:A:280:LEU:HD11	1:A:306:LEU:HD23	1.90	0.52
2:B:311:THR:HG23	2:B:333:LEU:HD23	1.92	0.51
1:A:451:GLN:NE2	12:A:4225:HOH:O	2.43	0.51
1:A:278[A]:HIS:CD2	1:A:339:ALA:HB1	2.46	0.51
4:H:165:LEU:HD21	4:H:187:VAL:HG21	1.93	0.51
2:B:63:VAL:HG23	2:B:63:VAL:O	2.11	0.51
5:L:136:LEU:N	5:L:136:LEU:HD12	2.24	0.51
4:H:177:GLN:NE2	12:H:4100:HOH:O	2.45	0.49
2:B:15:GLN:O	2:B:19:VAL:HG23	2.13	0.49
4:H:165:LEU:CD2	4:H:187:VAL:HG21	2.43	0.48
2:B:223:PHE:CZ	2:B:254:THR:HG21	2.49	0.48
2:B:142[B]:MET:SD	2:B:145:LEU:HD23	2.54	0.47
2:B:61:ALA:HB2	2:B:90:LEU:HD23	1.96	0.47
2:B:456:GLU:O	2:B:459:VAL:HG12	2.14	0.47
1:A:421:LEU:CD2	1:A:437:VAL:HG22	2.44	0.47
1:A:394:GLY:HA2	1:A:399:LEU:HD23	1.98	0.46
2:B:281:TYR:CE1	2:B:283:ALA:HB3	2.51	0.45
1:A:280:LEU:CD1	1:A:306:LEU:HD23	2.46	0.45
2:B:142[A]:MET:HE2	2:B:341:LEU:HG	1.98	0.45
4:H:156:VAL:CG2	4:H:183:LEU:HD13	2.47	0.45
1:A:122:ALA:O	1:A:123:GLU:HB2	2.16	0.44
4:H:183:LEU:HD23	4:H:183:LEU:C	2.38	0.44
1:A:307:LEU:HD21	1:A:330:LEU:HD13	1.98	0.44
4:H:12:VAL:CG2	4:H:86:LEU:HD13	2.47	0.44
5:L:37:GLN:HB2	5:L:47:LEU:HD11	1.99	0.44
5:L:195:GLU:HG2	5:L:206:VAL:HG22	1.99	0.44
4:H:172:PHE:CD1	5:L:164:THR:HG23	2.52	0.44
1:A:306:LEU:HD12	1:A:307:LEU:N	2.32	0.43
2:B:145:LEU:HD22	2:B:345:VAL:HG22	2.00	0.43
4:H:4:LEU:HD23	4:H:96:CYS:SG	2.58	0.43
1:A:379:PRO:HA	1:A:417:PHE:O	2.18	0.43
2:B:355:VAL:O	2:B:385:SER:HA	2.18	0.43
2:B:315:VAL:HG21	2:B:332:VAL:HG22	2.01	0.43
4:H:133:VAL:HG11	5:L:209:PHE:HB2	2.01	0.43
4:H:194:TRP:CG	4:H:195:PRO:HA	2.54	0.43
2:B:26:CYS:SG	2:B:31:LEU:HD22	2.58	0.42
1:A:390:LEU:HD12	1:A:390:LEU:N	2.34	0.42
5:L:105[B]:GLU:HG3	5:L:173:TYR:OH	2.19	0.42
4:H:133:VAL:HG12	4:H:134:CYS:H	1.85	0.42
1:A:122:ALA:O	1:A:123:GLU:CB	2.67	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:3:LEU:HG	1:A:366:LEU:HD21	2.02	0.41
2:B:355:VAL:HG23	2:B:389:LEU:HD22	2.03	0.41
1:A:427:ILE:HG22	1:A:434:ASP:OD1	2.20	0.41
1:A:213:LEU:HD13	4:H:103:TYR:CD2	2.55	0.41
2:B:308:PHE:CE2	2:B:328:THR:HG21	2.55	0.41
2:B:357:LEU:HD11	2:B:397:PHE:CD2	2.54	0.41
4:H:2:VAL:HG11	4:H:108:TYR:CD2	2.56	0.40
2:B:115:TYR:CZ	2:B:236:ILE:HD12	2.56	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	456/452 (101%)	443 (97%)	12 (3%)	1 (0%)	56	88
2	B	456/461 (99%)	427 (94%)	27 (6%)	2 (0%)	43	80
3	C	6/10 (60%)	5 (83%)	1 (17%)	0	100	100
4	H	217/221 (98%)	210 (97%)	7 (3%)	0	100	100
5	L	216/214 (101%)	211 (98%)	5 (2%)	0	100	100
All	All	1351/1358 (100%)	1296 (96%)	52 (4%)	3 (0%)	56	88

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	9	GLY
1	A	123	GLU
2	B	80	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	366/360 (102%)	358 (98%)	8 (2%)	64	92
2	B	410/409 (100%)	408 (100%)	2 (0%)	94	99
3	C	4/5 (80%)	4 (100%)	0	100	100
4	H	191/190 (100%)	189 (99%)	2 (1%)	85	98
5	L	192/188 (102%)	191 (100%)	1 (0%)	94	99
All	All	1163/1152 (101%)	1150 (99%)	13 (1%)	84	98

All (13) 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	197	GLN
1	A	221	LEU
1	A	264	LEU
1	A	288	TYR
1	A	413	THR
2	B	215	ASN
2	B	364	GLU
4	H	133	VAL
4	H	183	LEU
5	L	160	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	316	ASN
2	B	428	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	12,14,15	0.74	1 (8%)	15,19,21	0.89	1 (6%)
10	NAG	B	3321	10	12,14,15	0.79	1 (8%)	15,19,21	1.09	2 (13%)
10	MAN	B	3322	10	10,11,12	0.75	0	11,15,17	0.98	1 (9%)
10	MAN	B	3323	10	10,11,12	0.69	0	11,15,17	0.90	1 (9%)
10	MAN	B	3324	10	10,11,12	0.75	0	11,15,17	0.99	1 (9%)
11	NAG	B	3371	11,2	12,14,15	0.78	1 (8%)	15,19,21	0.64	0
11	NAG	B	3372	11	12,14,15	0.60	0	15,19,21	0.97	1 (6%)
11	MAN	B	3373	11	10,11,12	0.72	0	11,15,17	1.38	1 (9%)
11	MAN	B	3374	11	10,11,12	0.71	0	11,15,17	0.74	0
11	MAN	B	3375	11	10,11,12	0.79	0	11,15,17	0.72	0
11	MAN	B	3376	11	10,11,12	0.81	1 (10%)	11,15,17	1.14	1 (9%)
11	MAN	B	3377	11	10,11,12	0.71	0	11,15,17	0.97	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
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	1/1/4/5	0/2/19/22	0/1/1/1
10	MAN	B	3323	10	-	0/2/19/22	0/1/1/1
10	MAN	B	3324	10	-	0/2/19/22	0/1/1/1
11	NAG	B	3371	11,2	-	0/6/23/26	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	11	-	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	-	0/2/19/22	0/1/1/1
11	MAN	B	3377	11	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	3321	NAG	O5-C5	-2.53	1.40	1.45
11	B	3371	NAG	O5-C5	-2.40	1.41	1.45
10	B	3320	NAG	O5-C5	-2.24	1.41	1.45
11	B	3376	MAN	O5-C5	-2.04	1.41	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	3373	MAN	O5-C5-C6	4.01	111.19	106.98
11	B	3372	NAG	O5-C5-C6	2.79	109.90	106.98
10	B	3322	MAN	O5-C5-C6	2.73	109.84	106.98
10	B	3324	MAN	O5-C5-C6	2.68	109.79	106.98
11	B	3376	MAN	O5-C5-C6	2.66	109.77	106.98
10	B	3323	MAN	O5-C5-C6	2.58	109.69	106.98
10	B	3321	NAG	O5-C5-C4	-2.14	107.94	110.65
10	B	3321	NAG	C3-C2-N2	-2.09	108.59	111.76
10	B	3320	NAG	O4-C4-C3	-2.05	105.76	110.35

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	B	3322	MAN	C1
11	B	3373	MAN	C1

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

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	0.43	0	5,5,5	0.18	0
8	NAG	A	3015	1	12,14,15	0.61	0	15,19,21	1.16	1 (6%)
8	NAG	A	3249	1	12,14,15	0.60	0	15,19,21	0.91	0
6	GOL	B	1462	7	5,5,5	0.38	0	5,5,5	0.16	0
8	NAG	B	3099	2	12,14,15	0.73	1 (8%)	15,19,21	1.41	2 (13%)

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	1	-	0/6/23/26	0/1/1/1
8	NAG	A	3249	1	-	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	1/1/5/7	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	3099	NAG	O5-C5	-2.02	1.41	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	3015	NAG	O5-C5-C6	3.60	110.76	106.98
8	B	3099	NAG	O5-C5-C6	3.19	110.33	106.98
8	B	3099	NAG	O5-C5-C4	-2.68	107.25	110.65

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	B	3099	NAG	C1

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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%)	-0.07	8 (1%) 65 66	34, 51, 71, 85	2 (0%)
2	B	455/461 (98%)	0.34	43 (9%) 8 7	39, 63, 107, 121	3 (0%)
3	C	8/10 (80%)	1.36	2 (25%) 1 1	49, 79, 96, 102	0
4	H	219/221 (99%)	-0.20	3 (1%) 72 72	34, 52, 79, 110	1 (0%)
5	L	214/214 (100%)	-0.37	2 (0%) 81 81	32, 46, 64, 89	0
All	All	1348/1358 (99%)	0.01	58 (4%) 34 34	32, 54, 95, 121	6 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	451	GLY	8.0
2	B	448	CYS	6.8
2	B	453	GLY	6.5
5	L	214	CYS	5.9
2	B	444	ASN	5.6
2	B	454	THR	5.6
4	H	137	THR	5.6
2	B	443	PRO	5.6
3	C	405	ALA	5.5
4	H	221	PRO	5.2
2	B	450	ASN	5.2
2	B	460	CYS	5.1
2	B	35	SER	4.9
2	B	452	ASN	4.9
2	B	441	ALA	4.4
2	B	461	ARG	4.4
2	B	446	HIS	4.1
2	B	449	ASN	3.6
2	B	447	ARG	3.6
1	A	320	ARG	3.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	337[A]	PRO	3.5
2	B	445	SER	3.3
2	B	34	GLY	3.3
2	B	455	PHE	3.3
2	B	1	GLY	3.3
1	A	319	ASP	3.2
2	B	33	LEU	3.2
2	B	72	LYS	3.2
2	B	439	ALA	3.1
2	B	36	PRO	3.0
2	B	459	VAL	3.0
2	B	48	ASN	3.0
2	B	378	GLU	3.0
2	B	442	GLU	2.9
1	A	338	HIS	2.8
2	B	458	GLY	2.8
2	B	456	GLU	2.6
2	B	71	ASP	2.6
2	B	377	ASN	2.5
1	A	452	PRO	2.5
2	B	438	GLN	2.4
2	B	422	LYS	2.4
2	B	9	GLY	2.4
2	B	79	GLN	2.4
2	B	364	GLU	2.4
2	B	11	SER	2.4
4	H	220	GLY	2.3
2	B	408	GLN	2.3
2	B	409	GLU	2.3
5	L	212	ASN	2.3
3	C	406	LYS	2.2
1	A	292	SER	2.2
2	B	37	ARG	2.1
1	A	321	LYS	2.1
2	B	376	ASN	2.1
1	A	318	ALA	2.1
2	B	91	ARG	2.0
2	B	80	VAL	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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
11	MAN	B	3374	11/12	0.32	2.43	105,108,108,109	0
11	MAN	B	3373	11/12	0.20	0.42	87,99,101,104	0
11	MAN	B	3375	11/12	0.14	-0.15	76,81,86,90	0
11	NAG	B	3371	14/15	0.15	-0.49	78,82,86,89	0
11	MAN	B	3376	11/12	0.14	-0.77	64,68,72,72	0
10	NAG	B	3320	14/15	0.11	-2.98	60,64,69,77	0
10	MAN	B	3322	11/12	0.35	-	105,112,118,121	0
11	MAN	B	3377	11/12	0.34	-	93,94,95,95	0
11	NAG	B	3372	14/15	0.15	-	80,91,95,98	0
10	MAN	B	3324	11/12	0.39	-	120,122,123,123	0
10	MAN	B	3323	11/12	0.36	-	106,108,110,111	0
10	NAG	B	3321	14/15	0.24	-	82,86,93,101	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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	GOL	A	1453	6/6	0.30	3.05	69,70,73,75	0
8	NAG	B	3099	14/15	0.26	2.34	100,105,110,112	0
6	GOL	B	1462	6/6	0.19	2.29	68,71,72,72	0
7	CA	A	2005	1/1	0.12	-0.28	57,57,57,57	0
7	CA	A	2006	1/1	0.15	-0.32	66,66,66,66	0
7	CA	A	2004	1/1	0.12	-0.51	62,62,62,62	0
7	CA	B	2002	1/1	0.11	-0.95	49,49,49,49	0
7	CA	B	2003	1/1	0.16	-1.44	39,39,39,39	0
7	CA	A	2007	1/1	0.08	-2.15	63,63,63,63	0
9	MG	B	2001	1/1	0.12	-2.33	33,33,33,33	0
8	NAG	A	3015	14/15	0.36	-	93,95,96,96	14

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	NAG	A	3249	14/15	0.50	-	92,95,96,96	14

## 6.5 Other polymers ⓘ

There are no such residues in this entry.