



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:57 AM GMT

PDB ID : 2VDQ  
Title : INTEGRIN ALPHAIIIBBETA3 HEADPIECE BOUND TO A CHIMERIC  
FIBRINOGEN GAMMA CHAIN PEPTIDE, HHLGGAKQRGDV  
Authors : Springer, T.A.; Zhu, J.; Xiao, T.  
Deposited on : 2007-10-10  
Resolution : 2.59 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 (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

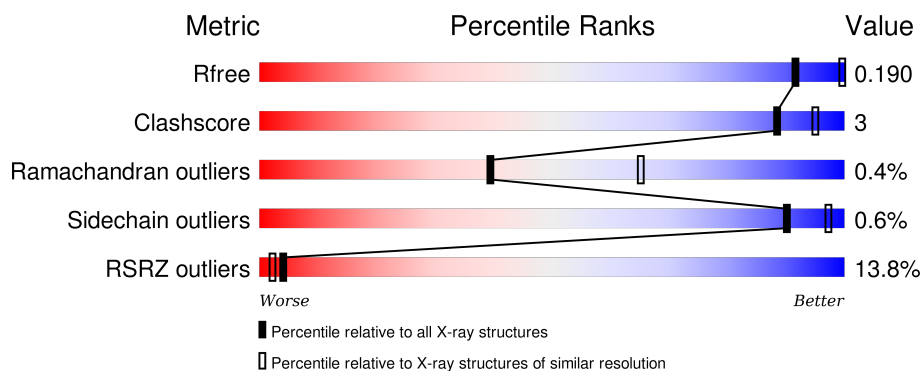
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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>10%</div> <div>96%</div> <div>.</div> </div>
2	B	461	<div> <div>24%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
3	C	12	<div> <div>17%</div> <div>58%</div> <div>42%</div> </div>
4	H	221	<div> <div>9%</div> <div>95%</div> <div>.</div> <div>.</div> </div>
5	L	214	<div> <div>3%</div> <div>93%</div> <div>7%</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	3322	X	-	-	-
11	MAN	B	3373	X	-	-	-
11	MAN	B	3374	-	-	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 12052 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	12	0
			3539	2250	616	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	9	0
			3571	2231	606	701	33			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	7	Total	C	N	O	0	0	0
			54	31	12	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	408	ARG	ALA	ENGINEERED MUTATION	UNP Q53Y18

- 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	4	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	8	0
			1679	1047	275	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		

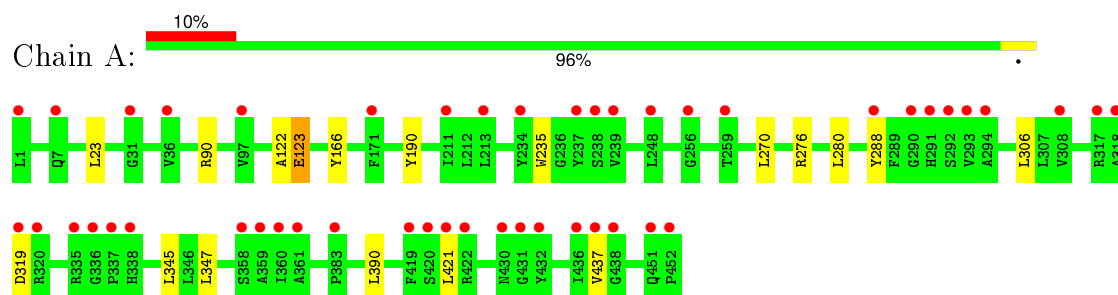
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	455	Total 455	O 455	0	0
12	B	335	Total 335	O 335	0	0
12	C	14	Total 14	O 14	0	0
12	H	247	Total 247	O 247	0	0
12	L	281	Total 281	O 281	0	0

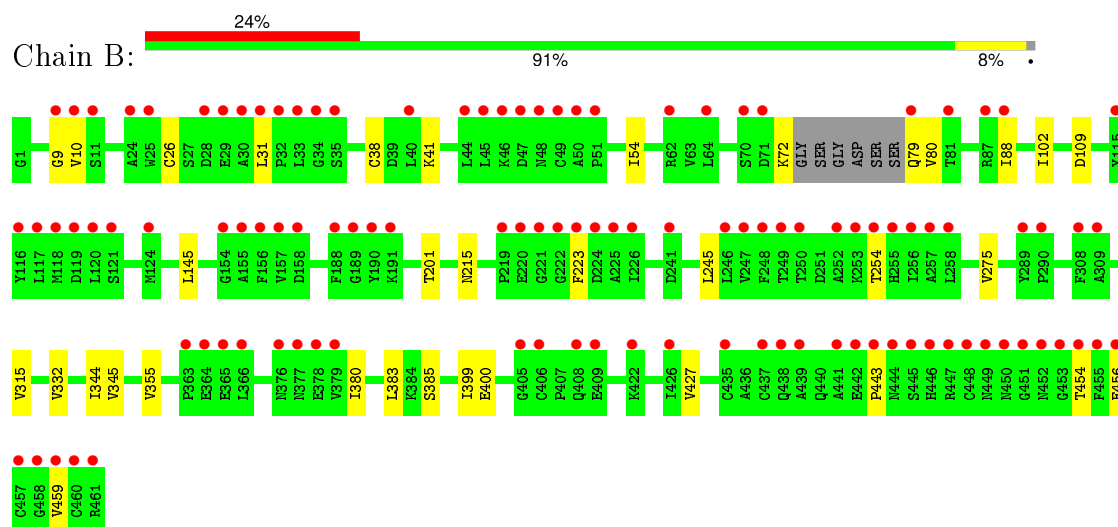
### 3 Residue-property plots

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



#### • Molecule 2: INTEGRIN BETA-3



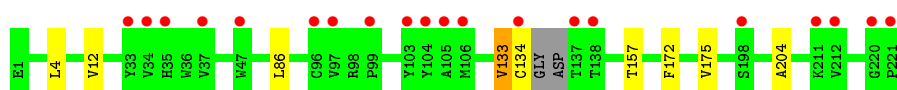
#### • Molecule 3: FIBRINOGEN, GAMMA POLYPEPTIDE



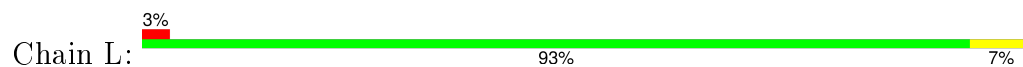
#### • Molecule 4: MONOCLONAL ANTIBODY 10E5 HEAVY CHAIN







● Molecule 5: MONOCLONAL ANTIBODY 10E5 LIGHT CHAIN



## 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)	34.63 – 2.59 34.63 – 2.59	Depositor EDS
% Data completeness (in resolution range)	92.2 (34.63-2.59) 90.8 (34.63-2.59)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.51 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, $R_{free}$	0.141 , 0.190 0.146 , 0.190	Depositor DCC
$R_{free}$ test set	3207 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.3	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 48.3	EDS
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 63490 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12052	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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, 0.375 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: 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	0/3656	0.55	0/4980
2	B	0.33	0/3652	0.50	0/4948
3	C	0.41	0/53	0.72	0/67
4	H	0.35	0/1721	0.53	0/2357
5	L	0.37	0/1744	0.55	0/2363
All	All	0.35	0/10826	0.53	0/14715

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 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	3539	0	3367	12	0
2	B	3571	0	3517	21	0
3	C	54	0	54	0	0
4	H	1672	0	1621	11	0
5	L	1679	0	1612	15	0
6	A	6	0	8	0	0
6	B	6	0	8	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	1	0
12	A	455	0	0	1	0
12	B	335	0	0	2	0
12	C	14	0	0	0	0
12	H	247	0	0	0	0
12	L	281	0	0	0	0
All	All	12052	0	10348	53	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 3.

All (53) 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:133:VAL:HG12	4:H:134:CYS:H	1.51	0.76
5:L:136:LEU:HD21	5:L:146:VAL:HG22	1.78	0.65
5:L:160[B]:LEU:HD12	5:L:161:ASN:N	2.12	0.64
2:B:88[B]:ILE:HD11	2:B:427:VAL:HG22	1.80	0.63
2:B:79:GLN:N	12:B:4037:HOH:O	2.33	0.60
1:A:270:LEU:HD23	1:A:276[A]:ARG:HA	1.85	0.59
1:A:270:LEU:HD23	1:A:276[B]:ARG:HA	1.86	0.58
2:B:443:PRO:HA	2:B:454:THR:HG22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:48:ILE:HD13	5:L:54:LEU:HD12	1.88	0.55
1:A:421:LEU:CD2	1:A:437:VAL:HG22	2.37	0.54
4:H:175:VAL:HG11	5:L:160[B]:LEU:CD1	2.38	0.53
5:L:136:LEU:N	5:L:136:LEU:HD12	2.22	0.53
1:A:280:LEU:HD11	1:A:306:LEU:HD23	1.89	0.53
2:B:145:LEU:HD22	2:B:345:VAL:HG22	1.90	0.53
4:H:175:VAL:HG11	5:L:160[B]:LEU:HD11	1.90	0.53
1:A:235:TRP:CZ2	1:A:270:LEU:HD11	2.46	0.51
4:H:175:VAL:CB	5:L:160[B]:LEU:HD11	2.40	0.51
5:L:105[A]:GLU:HG3	5:L:173:TYR:OH	2.11	0.51
1:A:280:LEU:CD1	1:A:306:LEU:HD23	2.41	0.50
2:B:456:GLU:O	2:B:459:VAL:HG12	2.13	0.48
2:B:245:LEU:CD1	2:B:344:ILE:HG23	2.44	0.48
2:B:315:VAL:HG21	2:B:332:VAL:HG22	1.96	0.48
2:B:72:LYS:NZ	2:B:109:ASP:OD1	2.46	0.48
1:A:90[A]:ARG:CZ	12:A:4131:HOH:O	2.62	0.47
2:B:10:VAL:HG23	2:B:10:VAL:O	2.15	0.46
1:A:122:ALA:O	1:A:123:GLU:HB2	2.16	0.45
4:H:172:PHE:CD1	5:L:164:THR:HG23	2.51	0.45
4:H:157:THR:OG1	4:H:204:ALA:HB3	2.17	0.45
4:H:175:VAL:CG1	5:L:160[B]:LEU:HD11	2.47	0.44
2:B:10:VAL:HG11	2:B:38:CYS:SG	2.57	0.44
2:B:223:PHE:CZ	2:B:254:THR:HG21	2.53	0.44
1:A:390:LEU:HD12	1:A:390:LEU:N	2.33	0.44
2:B:201[A]:THR:HG23	12:B:4129:HOH:O	2.18	0.44
4:H:175:VAL:HB	5:L:160[B]:LEU:HD11	1.99	0.44
2:B:245:LEU:HD13	2:B:344:ILE:HD12	2.00	0.43
5:L:122:SER:O	5:L:126:THR:HG23	2.19	0.43
5:L:195:GLU:HG2	5:L:206:VAL:HG22	2.00	0.43
5:L:150:ILE:HD12	5:L:155[A]:ARG:HD3	1.99	0.42
1:A:235:TRP:HZ2	1:A:270:LEU:HD11	1.84	0.42
2:B:399:ILE:N	2:B:399:ILE:HD12	2.34	0.42
2:B:88[B]:ILE:CG1	2:B:427:VAL:HG22	2.49	0.42
2:B:26:CYS:SG	2:B:31:LEU:HD22	2.59	0.42
4:H:133:VAL:HG12	4:H:134:CYS:N	2.28	0.42
2:B:355:VAL:O	2:B:385:SER:HA	2.20	0.42
2:B:88[B]:ILE:CD1	2:B:427:VAL:HG22	2.47	0.42
5:L:105[A]:GLU:HG3	5:L:173:TYR:HH	1.85	0.41
2:B:41:LYS:HG3	2:B:54:ILE:HG21	2.02	0.41
1:A:280:LEU:CD1	1:A:306:LEU:CD2	2.99	0.41
2:B:400:GLU:HB2	11:B:3371:NAG:H83	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:12:VAL:HG21	4:H:86:LEU:HD13	2.02	0.40
1:A:345:LEU:HD21	1:A:347:LEU:HD21	2.04	0.40
2:B:380:ILE:HG21	2:B:383:LEU:HD22	2.03	0.40
4:H:4:LEU:N	4:H:4:LEU:HD12	2.36	0.40

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	459/452 (102%)	447 (97%)	11 (2%)	1 (0%)	52	77
2	B	459/461 (100%)	438 (95%)	18 (4%)	3 (1%)	26	51
3	C	5/12 (42%)	5 (100%)	0	0	100	100
4	H	217/221 (98%)	212 (98%)	4 (2%)	1 (0%)	34	60
5	L	221/214 (103%)	216 (98%)	5 (2%)	0	100	100
All	All	1361/1360 (100%)	1318 (97%)	38 (3%)	5 (0%)	39	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
2	B	9	GLY
4	H	133	VAL
2	B	80	VAL
2	B	275	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	369/360 (102%)	364 (99%)	5 (1%)	74	90
2	B	413/409 (101%)	411 (100%)	2 (0%)	92	98
3	C	5/8 (62%)	5 (100%)	0	100	100
4	H	191/190 (100%)	191 (100%)	0	100	100
5	L	197/188 (105%)	197 (100%)	0	100	100
All	All	1175/1155 (102%)	1168 (99%)	7 (1%)	90	97

All (7) 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
1	A	319	ASP
2	B	102	ILE
2	B	215	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	316	ASN
2	B	428	GLN
2	B	438	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	0.55	0	15,19,21	0.77	0
10	NAG	B	3321	10	14,14,15	0.70	0	15,19,21	0.99	2 (13%)
10	MAN	B	3322	10	11,11,12	0.57	0	14,15,17	0.77	0
10	MAN	B	3323	10	11,11,12	0.53	0	14,15,17	0.74	0
10	MAN	B	3324	10	11,11,12	0.68	0	14,15,17	1.51	2 (14%)
11	NAG	B	3371	11,2	14,14,15	0.67	0	15,19,21	0.74	0
11	NAG	B	3372	11	14,14,15	0.51	0	15,19,21	0.96	0
11	MAN	B	3373	11	11,11,12	0.54	0	14,15,17	0.87	0
11	MAN	B	3374	11	11,11,12	0.57	0	14,15,17	0.83	0
11	MAN	B	3375	11	11,11,12	0.53	0	14,15,17	1.31	1 (7%)
11	MAN	B	3376	11	11,11,12	0.51	0	14,15,17	1.01	1 (7%)
11	MAN	B	3377	11	11,11,12	0.56	0	14,15,17	0.95	1 (7%)

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
11	NAG	B	3372	11	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	3321	NAG	C3-C4-C5	2.08	113.83	110.20
10	B	3321	NAG	C4-C3-C2	2.21	114.67	111.23
11	B	3377	MAN	C1-O5-C5	2.27	115.13	112.25
10	B	3324	MAN	C1-O5-C5	2.35	115.23	112.25
11	B	3376	MAN	C1-O5-C5	2.78	115.78	112.25
11	B	3375	MAN	C1-O5-C5	4.12	117.48	112.25
10	B	3324	MAN	C1-C2-C3	4.39	114.73	109.54

All (2) chirality outliers are listed below:

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

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	3371	NAG	1	0

## 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	0.42	0	5,5,5	0.10	0
8	NAG	A	3015	1	14,14,15	0.46	0	15,19,21	0.82	1 (6%)
8	NAG	A	3249	1	14,14,15	0.52	0	15,19,21	0.81	0
6	GOL	B	1462	7	5,5,5	0.36	0	5,5,5	0.40	0
8	NAG	B	3099	2	14,14,15	0.44	0	15,19,21	0.70	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
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	-	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	A	3015	NAG	C1-O5-C5	2.10	114.91	112.25

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%)	0.73	47 (10%) 8 5	31, 46, 62, 87	3 (0%)
2	B	455/461 (98%)	1.29	111 (24%) 1 0	36, 56, 93, 106	0
3	C	7/12 (58%)	1.02	2 (28%) 1 0	39, 48, 108, 111	0
4	H	219/221 (99%)	0.71	20 (9%) 11 7	32, 46, 73, 105	2 (0%)
5	L	214/214 (100%)	0.40	6 (2%) 56 49	31, 45, 57, 92	0
All	All	1347/1360 (99%)	0.86	186 (13%) 4 2	31, 48, 85, 111	5 (0%)

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	454	THR	8.7
2	B	448	CYS	8.7
2	B	443	PRO	8.7
4	H	137	THR	8.7
2	B	453	GLY	8.6
2	B	451	GLY	8.5
2	B	444	ASN	8.1
2	B	452	ASN	7.7
4	H	221	PRO	6.9
5	L	214	CYS	6.8
2	B	11	SER	6.0
1	A	320[A]	ARG	6.0
2	B	460	CYS	5.9
2	B	33	LEU	5.7
2	B	48	ASN	5.6
2	B	450	ASN	5.6
1	A	337	PRO	5.6
2	B	445	SER	5.4
2	B	117	LEU	5.3
2	B	30	ALA	5.3

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Mol	Chain	Res	Type	RSRZ
2	B	461	ARG	5.1
2	B	156	PHE	5.1
1	A	319	ASP	4.9
3	C	405	ALA	4.8
4	H	138	THR	4.8
2	B	34	GLY	4.8
2	B	459	VAL	4.7
2	B	449	ASN	4.7
1	A	318	ALA	4.6
2	B	446	HIS	4.6
2	B	455	PHE	4.6
2	B	221	GLY	4.5
2	B	35	SER	4.5
4	H	220	GLY	4.4
2	B	248	PHE	4.4
2	B	405	GLY	4.4
2	B	249	THR	4.4
2	B	225	ALA	4.3
2	B	31	LEU	4.3
2	B	10	VAL	4.3
2	B	28	ASP	4.3
2	B	120	LEU	4.2
4	H	134	CYS	4.1
2	B	441	ALA	4.1
2	B	223	PHE	4.1
1	A	452	PRO	4.1
2	B	157	VAL	4.0
2	B	447	ARG	4.0
1	A	421	LEU	4.0
2	B	155	ALA	3.9
2	B	32	PRO	3.9
2	B	378	GLU	3.8
2	B	79	GLN	3.8
4	H	106	MET	3.8
2	B	24	ALA	3.7
2	B	118	MET	3.5
2	B	247	VAL	3.5
2	B	226	ILE	3.5
2	B	376	ASN	3.5
2	B	45	LEU	3.5
2	B	222	GLY	3.4
2	B	408	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
5	L	91	TYR	3.4
2	B	246	LEU	3.4
1	A	237	TYR	3.4
2	B	256	ILE	3.4
2	B	29	GLU	3.4
2	B	47	ASP	3.4
4	H	105	ALA	3.3
1	A	358	SER	3.3
2	B	51	PRO	3.3
4	H	198	SER	3.2
1	A	31	GLY	3.2
1	A	292[A]	SER	3.2
1	A	361	ALA	3.2
2	B	154	GLY	3.2
1	A	359	ALA	3.1
2	B	115	TYR	3.1
1	A	338	HIS	3.1
2	B	49	CYS	3.1
2	B	435	CYS	3.1
1	A	335[A]	ARG	3.1
2	B	62	ARG	3.1
2	B	364	GLU	3.1
1	A	436	ILE	3.1
2	B	422	LYS	3.0
2	B	70	SER	3.0
1	A	336	GLY	3.0
2	B	119	ASP	2.9
1	A	290	GLY	2.9
1	A	422	ARG	2.9
2	B	255	HIS	2.9
1	A	291	HIS	2.9
1	A	293	VAL	2.8
4	H	35	HIS	2.8
2	B	409	GLU	2.8
2	B	250	THR	2.8
2	B	188	PHE	2.8
1	A	294	ALA	2.8
4	H	34	VAL	2.8
2	B	81	THR	2.8
4	H	104	TYR	2.8
5	L	201	SER	2.8
2	B	379	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
4	H	33	TYR	2.7
2	B	252	ALA	2.7
1	A	383	PRO	2.7
2	B	254	THR	2.7
2	B	442	GLU	2.7
2	B	71	ASP	2.6
2	B	258	LEU	2.6
1	A	360	ILE	2.6
1	A	259	THR	2.6
2	B	189	GLY	2.6
1	A	213	LEU	2.6
4	H	103	TYR	2.6
5	L	202	THR	2.6
1	A	97	VAL	2.5
4	H	212	VAL	2.5
2	B	241	ASP	2.5
1	A	420	SER	2.5
2	B	190	TYR	2.5
2	B	46	LYS	2.5
2	B	377	ASN	2.5
2	B	289	TYR	2.5
2	B	9	GLY	2.5
4	H	97	VAL	2.5
2	B	219	PRO	2.5
1	A	419	PHE	2.5
2	B	438	GLN	2.5
1	A	432	TYR	2.5
2	B	456	GLU	2.5
2	B	457	CYS	2.4
2	B	40	LEU	2.4
1	A	234	TYR	2.4
1	A	239	VAL	2.4
1	A	317	ARG	2.4
1	A	431	GLY	2.4
2	B	50	ALA	2.4
1	A	288	TYR	2.3
1	A	248	LEU	2.3
2	B	191	LYS	2.3
2	B	121	SER	2.3
1	A	451	GLN	2.3
3	C	406	LYS	2.3
2	B	124	MET	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	253	LYS	2.3
1	A	238	SER	2.2
2	B	44	LEU	2.2
2	B	439	ALA	2.2
2	B	426	ILE	2.2
2	B	308	PHE	2.2
2	B	88[A]	ILE	2.2
1	A	1	LEU	2.2
2	B	363	PRO	2.2
1	A	437	VAL	2.2
2	B	257	ALA	2.2
2	B	309	ALA	2.2
4	H	99	PRO	2.2
4	H	211	LYS	2.2
2	B	406	CYS	2.2
1	A	171	PHE	2.2
1	A	430	ASN	2.2
2	B	224	ASP	2.2
2	B	220	GLU	2.1
1	A	438	GLY	2.1
2	B	365	GLU	2.1
2	B	458	GLY	2.1
1	A	308	VAL	2.1
2	B	158	ASP	2.1
2	B	116	TYR	2.1
1	A	256	GLY	2.1
2	B	290	PRO	2.1
2	B	437	CYS	2.1
4	H	47	TRP	2.1
1	A	211	ILE	2.1
5	L	96	TYR	2.1
2	B	366	LEU	2.1
2	B	64	LEU	2.1
1	A	7	GLN	2.0
2	B	87	ARG	2.0
1	A	36[A]	VAL	2.0
2	B	25	TRP	2.0
4	H	96	CYS	2.0
4	H	37	VAL	2.0
5	L	36	LEU	2.0

## 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, 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	0.90	0.38	11.77	98,101,102,103	0
11	NAG	B	3371	14/15	0.91	0.19	0.22	66,75,78,80	0
11	MAN	B	3375	11/12	0.94	0.33	-	70,77,82,88	0
11	MAN	B	3376	11/12	0.92	0.19	-	61,66,70,71	0
10	MAN	B	3324	11/12	0.73	0.52	-	119,120,121,121	0
10	NAG	B	3320	14/15	0.94	0.24	-	50,56,63,71	0
10	NAG	B	3321	14/15	0.93	0.42	-	77,81,88,96	0
10	MAN	B	3323	11/12	0.87	0.45	-	103,107,109,109	0
11	MAN	B	3373	11/12	0.85	0.34	-	83,93,95,98	0
11	NAG	B	3372	14/15	0.89	0.28	-	67,83,89,93	0
11	MAN	B	3377	11/12	0.87	0.38	-	91,93,94,95	0
10	MAN	B	3322	11/12	0.73	0.45	-	103,109,114,118	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, 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	A	1453	6/6	0.92	0.20	0.45	58,64,68,72	0
6	GOL	B	1462	6/6	0.95	0.15	-0.70	54,55,57,58	0
7	CA	A	2004	1/1	0.97	0.13	-0.86	58,58,58,58	0
7	CA	A	2005	1/1	0.94	0.11	-1.69	49,49,49,49	0
7	CA	A	2007	1/1	0.96	0.11	-1.78	57,57,57,57	0
7	CA	A	2006	1/1	0.97	0.11	-2.46	64,64,64,64	0
9	MG	B	2001	1/1	0.95	0.05	-2.63	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	CA	B	2002	1/1	0.99	0.04	-3.14	35,35,35,35	0
7	CA	B	2003	1/1	0.99	0.03	-4.74	34,34,34,34	0
8	NAG	B	3099	14/15	0.81	0.47	-	99,105,111,112	0
8	NAG	A	3249	14/15	0.48	0.65	-	98,102,104,105	14
8	NAG	A	3015	14/15	0.75	0.49	-	90,95,97,97	14

## 6.5 Other polymers [i](#)

There are no such residues in this entry.