



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:56 AM GMT

PDB ID : 2VC2  
Title : RE-REFINEMENT OF INTEGRIN ALPHAIIIBBETA3 HEADPIECE  
BOUND TO ANTAGONIST L-739758  
Authors : Springer, T.A.; Zhu, J.; Xiao, T.  
Deposited on : 2007-09-18  
Resolution : 3.10 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

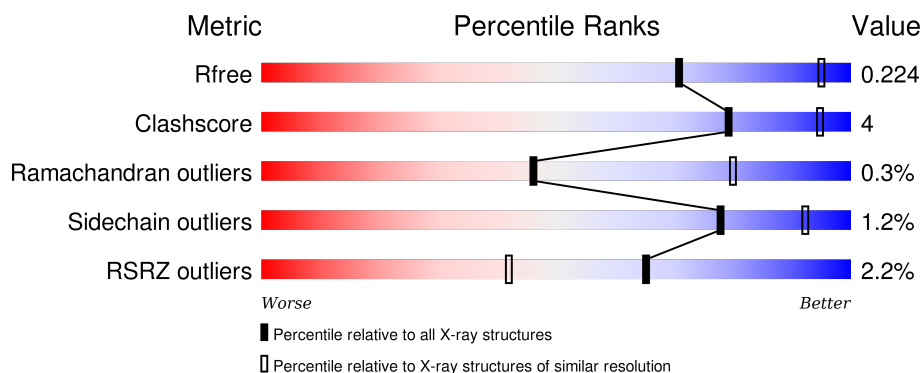
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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></div> <div>91% 9%</div> </div>
2	B	461	<div> <div>5%</div> <div>87% 11%</div> </div>
3	H	221	<div> <div></div> <div>90% 10%</div> </div>
4	L	214	<div> <div></div> <div>94% 6%</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	-	-	-
6	GOL	B	1478	-	-	-	X
9	180	B	1477	X	-	-	-

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 10686 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	3	0
			3493	2218	606	661	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	282	GLY	ALA	SEE REMARK 999	UNP P08514

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	457	Total	C	N	O	S	0	2	0
			3543	2208	606	697	32			

- Molecule 3 is a protein called MONOCLONAL ANTIBODY 10E5 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	219	Total	C	N	O	S	0	2	0
			1675	1061	271	337	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	214	Total	C	N	O	S	0	1	0
			1637	1019	268	341	9			

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

- 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).

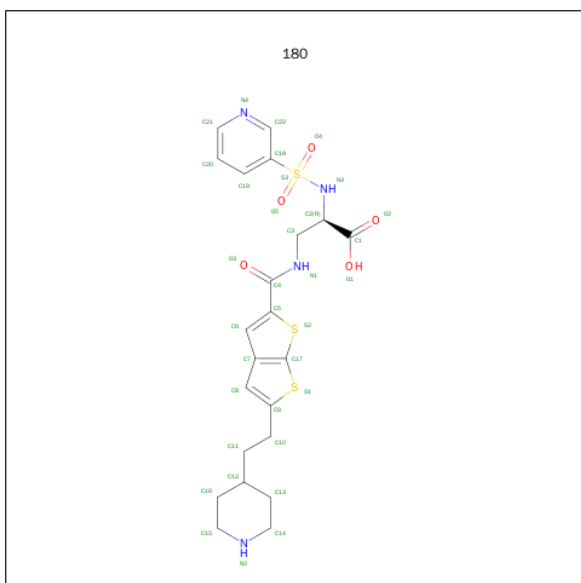
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Ca	0	0
			2	2		
7	A	4	Total	Ca	0	0
			4	4		

- 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 2-(S)-[N-(3-PYRIDYLSULFONYL)AMINO]-3-[[2-CARBONYL-5-[2-(PIPERIDIN-4-YL)ETHYL]-THIENO[2,3-B]THIOPHENEYL]AMINO]-PROPIONIC ACID (three-letter code: 180) (formula: C<sub>22</sub>H<sub>26</sub>N<sub>4</sub>O<sub>5</sub>S<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			34	22	4	5	3		

- 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		

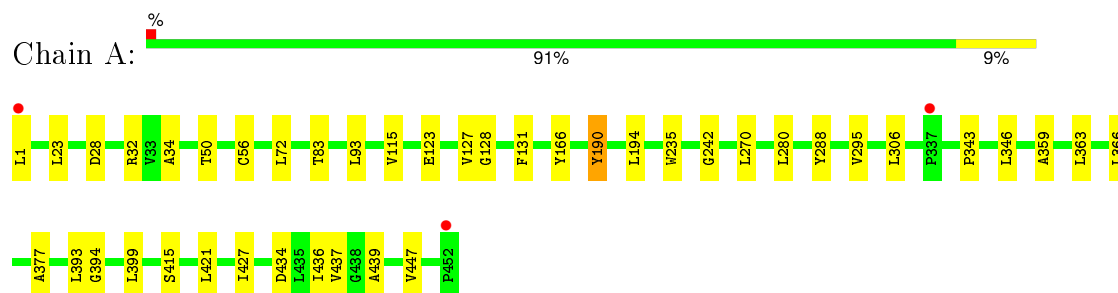
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	33	Total	O	0	0
			33	33		
12	B	26	Total	O	0	0
			26	26		
12	H	22	Total	O	0	0
			22	22		
12	L	17	Total	O	0	0
			17	17		

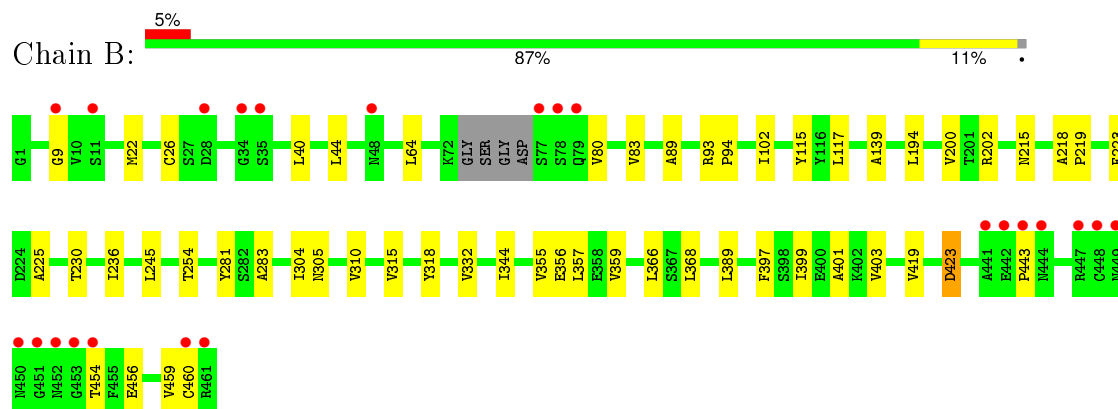
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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.

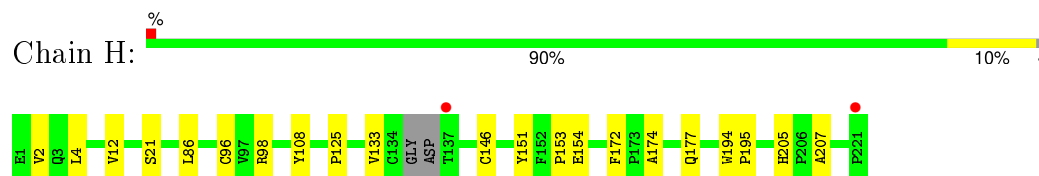
#### • Molecule 1: INTEGRIN ALPHA-IIB



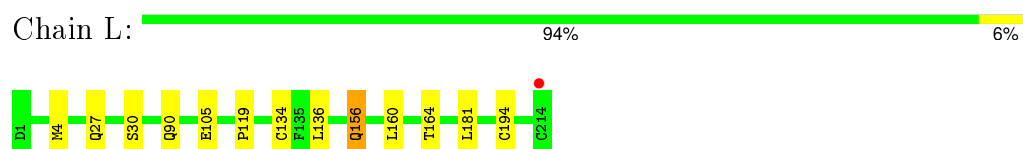
#### • Molecule 2: INTEGRIN BETA-3



#### • Molecule 3: MONOCLONAL ANTIBODY 10E5 HEAVY CHAIN



#### • Molecule 4: 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, $\alpha$ , $\beta$ , $\gamma$	149.15Å 149.15Å 176.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.72 – 3.10 42.70 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.7 (42.72-3.10) 94.8 (42.70-3.10)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, $R_{free}$	0.177 , 0.217 0.190 , 0.224	Depositor DCC
$R_{free}$ test set	1985 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.4	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 24.8	EDS
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 39430 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10686	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	3.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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, NAG, CA, 180, 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	0.33	0/3596	0.52	0/4899
2	B	0.32	0/3607	0.49	0/4889
3	H	0.33	0/1721	0.49	0/2356
4	L	0.32	0/1673	0.52	0/2269
All	All	0.32	0/10597	0.51	0/14413

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	3493	0	3329	24	0
2	B	3543	0	3470	30	0
3	H	1675	0	1630	16	0
4	L	1637	0	1551	6	0
5	A	1	0	0	0	0
5	B	1	0	0	0	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	34	0	25	2	0
10	B	61	0	52	0	0
11	B	83	0	70	0	0
12	A	33	0	0	0	0
12	B	26	0	0	0	0
12	H	22	0	0	1	0
12	L	17	0	0	0	0
All	All	10686	0	10181	73	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 4.

All (73) 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:B:230:THR:HG23	2:B:304:ILE:HD12	1.65	0.77
2:B:359:VAL:HG21	2:B:368:LEU:HD12	1.74	0.69
2:B:117:LEU:HD22	2:B:225:ALA:HB1	1.76	0.67
2:B:26:CYS:HB2	2:B:44:LEU:HD22	1.80	0.63
1:A:190:TYR:CE1	9:B:1477:180:H8	2.37	0.59
1:A:235:TRP:CZ2	1:A:270:LEU:HD11	2.39	0.58
2:B:443:PRO:HA	2:B:454:THR:HG22	1.85	0.57
3:H:205:HIS:CE1	3:H:207:ALA:HB3	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:TRP:HZ2	1:A:270:LEU:HD11	1.70	0.57
3:H:12:VAL:HG21	3:H:86:LEU:HD13	1.88	0.56
2:B:355:VAL:HG23	2:B:389:LEU:HD22	1.88	0.56
1:A:427:ILE:HG22	1:A:434:ASP:OD1	2.07	0.54
3:H:2:VAL:HG11	3:H:108:TYR:CD2	2.42	0.54
1:A:190:TYR:CD1	9:B:1477:180:H8	2.43	0.53
3:H:12:VAL:CG2	3:H:86:LEU:HD13	2.40	0.51
3:H:172:PHE:CD1	4:L:164:THR:HG23	2.45	0.51
1:A:359:ALA:HB3	1:A:377:ALA:HB3	1.91	0.51
4:L:181:LEU:N	4:L:181:LEU:HD23	2.25	0.51
2:B:281:TYR:CE1	2:B:283:ALA:HB3	2.46	0.51
2:B:245:LEU:HD13	2:B:344:ILE:HG23	1.92	0.51
2:B:102:ILE:HG21	2:B:399:ILE:HD11	1.92	0.49
1:A:34:ALA:HB1	1:A:56:CYS:O	2.12	0.49
1:A:359:ALA:HB3	1:A:377:ALA:CB	2.43	0.49
2:B:356:GLU:O	2:B:419:VAL:HG23	2.13	0.49
4:L:4:MET:HE2	4:L:90:GLN:HB3	1.94	0.48
2:B:368:LEU:CD2	2:B:401:ALA:HB2	2.43	0.48
2:B:310:VAL:HG11	2:B:318:TYR:CD2	2.49	0.48
1:A:415:SER:HB2	1:A:439:ALA:HB1	1.96	0.48
2:B:456:GLU:O	2:B:459:VAL:HG12	2.15	0.47
3:H:154:GLU:OE2	3:H:174:ALA:HB3	2.14	0.47
1:A:363:LEU:HD13	1:A:366:LEU:HD22	1.96	0.47
3:H:4:LEU:HD23	3:H:96:CYS:SG	2.55	0.47
3:H:177[B]:GLN:OE1	4:L:160:LEU:HD13	2.14	0.47
3:H:153:PRO:HD2	3:H:207:ALA:CB	2.45	0.47
2:B:245:LEU:HD23	2:B:305:ASN:HB2	1.97	0.46
1:A:1:LEU:HB2	1:A:393:LEU:HD11	1.96	0.46
1:A:93:LEU:HD13	1:A:131:PHE:CD1	2.52	0.45
1:A:394:GLY:HA2	1:A:399:LEU:HD23	1.97	0.45
1:A:421:LEU:CD2	1:A:437:VAL:HG22	2.46	0.44
1:A:280:LEU:HD11	1:A:306:LEU:HD23	1.99	0.44
2:B:83:VAL:HG23	2:B:423:ASP:HB2	1.98	0.44
1:A:50:THR:OG1	1:A:72:LEU:HD13	2.18	0.44
2:B:64:LEU:HD11	2:B:89:ALA:HB2	1.99	0.44
4:L:156:GLN:HE21	4:L:156:GLN:HA	1.82	0.44
2:B:218:ALA:HB3	2:B:219:PRO:HD3	1.98	0.44
2:B:115:TYR:CZ	2:B:236:ILE:HD12	2.52	0.44
3:H:177[A]:GLN:NE2	12:H:4021:HOH:O	2.51	0.44
2:B:355:VAL:HG23	2:B:389:LEU:CD2	2.48	0.44
1:A:343:PRO:HG2	1:A:346:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:ALA:HB1	2:B:200:VAL:HG13	2.00	0.44
2:B:315:VAL:HG21	2:B:332:VAL:HG22	2.00	0.43
3:H:125:PRO:HB3	3:H:151:TYR:HB3	2.00	0.43
3:H:98:ARG:HG3	3:H:108:TYR:HB2	1.99	0.43
3:H:153:PRO:HD2	3:H:207:ALA:HB1	2.00	0.43
2:B:223:PHE:CZ	2:B:254:THR:HG21	2.54	0.43
2:B:366:LEU:HD23	2:B:403:VAL:HA	1.99	0.43
2:B:357:LEU:HD11	2:B:397:PHE:CG	2.54	0.43
2:B:194:LEU:HD11	2:B:202:ARG:HE	1.84	0.42
3:H:205:HIS:NE2	3:H:207:ALA:HB3	2.34	0.42
2:B:459:VAL:HG22	2:B:460:CYS:O	2.18	0.42
1:A:242:GLY:HA3	1:A:295:VAL:HG11	2.01	0.42
1:A:377:ALA:HB2	1:A:421:LEU:HD11	2.01	0.42
1:A:194:LEU:HD12	1:A:194:LEU:C	2.41	0.41
2:B:102:ILE:CG2	2:B:399:ILE:HD11	2.49	0.41
3:H:133:VAL:HG22	4:L:119:PRO:HD3	2.01	0.41
2:B:22:MET:HE2	2:B:40:LEU:HD22	2.02	0.41
1:A:28:ASP:OD2	1:A:32:ARG:HB3	2.20	0.41
1:A:127:VAL:HG23	1:A:128:GLY:O	2.20	0.41
3:H:194:TRP:CG	3:H:195:PRO:HA	2.56	0.41
2:B:93:ARG:HB2	2:B:94:PRO:HD2	2.03	0.41
1:A:83:THR:O	1:A:115:VAL:HA	2.21	0.41
2:B:223:PHE:CE1	2:B:254:THR:HG21	2.56	0.40
1:A:436:ILE:HG22	1:A:447:VAL:HG22	2.03	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	453/452 (100%)	436 (96%)	16 (4%)	1 (0%)	52 84

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	454/461 (98%)	425 (94%)	27 (6%)	2 (0%)	39	75
3	H	217/221 (98%)	211 (97%)	6 (3%)	0	100	100
4	L	212/214 (99%)	202 (95%)	9 (4%)	1 (0%)	34	72
All	All	1336/1348 (99%)	1274 (95%)	58 (4%)	4 (0%)	46	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	9	GLY
4	L	30	SER
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	363/360 (101%)	359 (99%)	4 (1%)	80	93
2	B	408/409 (100%)	406 (100%)	2 (0%)	92	96
3	H	191/190 (100%)	189 (99%)	2 (1%)	82	93
4	L	188/188 (100%)	182 (97%)	6 (3%)	46	79
All	All	1150/1147 (100%)	1136 (99%)	14 (1%)	78	92

All (14) 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	423	ASP
3	H	21	SER

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Mol	Chain	Res	Type
3	H	146	CYS
4	L	27	GLN
4	L	105	GLU
4	L	134	CYS
4	L	136	LEU
4	L	156	GLN
4	L	194[A]	CYS

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	342	GLN
2	B	428	GLN
4	L	156	GLN

### 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](#)

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	0.57	0	15,19,21	0.69	0
10	NAG	B	3321	10	14,14,15	0.62	0	15,19,21	0.79	0
10	MAN	B	3322	10	11,11,12	0.60	0	14,15,17	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	MAN	B	3323	10	11,11,12	0.51	0	14,15,17	0.83	1 (7%)
10	MAN	B	3324	10	11,11,12	0.58	0	14,15,17	1.51	2 (14%)
11	NAG	B	3371	11,2	14,14,15	0.58	0	15,19,21	0.69	0
11	NAG	B	3372	11	14,14,15	0.48	0	15,19,21	0.88	0
11	MAN	B	3373	11	11,11,12	0.64	0	14,15,17	1.01	1 (7%)
11	MAN	B	3374	11	11,11,12	0.56	0	14,15,17	0.82	0
11	MAN	B	3375	11	11,11,12	0.57	0	14,15,17	1.19	1 (7%)
11	MAN	B	3376	11	11,11,12	0.56	0	14,15,17	1.53	2 (14%)
11	MAN	B	3377	11	11,11,12	0.61	0	14,15,17	1.36	2 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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 (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	3373	MAN	O5-C1-C2	-2.15	107.37	110.86
10	B	3323	MAN	C1-O5-C5	2.18	115.01	112.25
11	B	3377	MAN	C1-O5-C5	2.74	115.73	112.25
11	B	3376	MAN	C1-O5-C5	2.93	115.97	112.25
10	B	3324	MAN	C1-O5-C5	2.96	116.01	112.25
11	B	3377	MAN	C3-C4-C5	3.04	115.50	110.20
11	B	3375	MAN	C1-O5-C5	3.54	116.74	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	3376	MAN	C1-C2-C3	3.79	114.03	109.54
10	B	3324	MAN	C1-C2-C3	3.84	114.08	109.54

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.

No monomer is involved in short contacts.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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	1461	-	5,5,5	0.35	0	5,5,5	0.21	0
8	NAG	A	3015	1	14,14,15	0.67	0	15,19,21	1.79	1 (6%)
8	NAG	A	3249	1	14,14,15	0.60	0	15,19,21	0.77	0
9	180	B	1477	5	27,37,37	2.26	5 (18%)	26,52,52	2.17	4 (15%)
6	GOL	B	1478	7	5,5,5	0.34	0	5,5,5	0.26	0
8	NAG	B	3099	2	14,14,15	0.56	0	15,19,21	0.80	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	1461	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
9	180	B	1477	5	1/1/5/8	0/22/37/37	0/4/4/4
6	GOL	B	1478	7	-	0/4/4/4	0/0/0/0
8	NAG	B	3099	2	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1477	180	C5-S2	-6.11	1.64	1.72
9	B	1477	180	C9-S1	-5.05	1.64	1.74
9	B	1477	180	C18-S3	-2.16	1.73	1.76
9	B	1477	180	O4-S3	5.38	1.49	1.43
9	B	1477	180	O5-S3	5.80	1.49	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	1477	180	O5-S3-O4	-8.30	108.52	119.54
9	B	1477	180	C18-C22-N4	-3.96	120.39	123.51
9	B	1477	180	C21-N4-C22	2.82	122.04	116.84
9	B	1477	180	C18-S3-N3	3.42	112.62	107.71
8	A	3015	NAG	C1-O5-C5	6.07	119.95	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	B	1477	180	C2

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	1477	180	2	0

## 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%)	-0.57	3 (0%) 89 78	2, 2, 7, 19	1 (0%)
2	B	457/461 (99%)	-0.05	23 (5%) 32 13	2, 2, 9, 17	1 (0%)
3	H	219/221 (99%)	-0.45	2 (0%) 85 72	2, 2, 8, 23	0
4	L	214/214 (100%)	-0.55	1 (0%) 91 83	2, 2, 7, 11	1 (0%)
All	All	1342/1348 (99%)	-0.37	29 (2%) 65 42	2, 2, 8, 23	3 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	444	ASN	4.4
3	H	137	THR	4.1
1	A	337	PRO	4.0
2	B	443	PRO	3.8
2	B	11	SER	3.6
2	B	450	ASN	3.5
2	B	454	THR	3.5
2	B	451	GLY	3.3
3	H	221	PRO	3.2
2	B	448	CYS	3.2
4	L	214	CYS	3.0
2	B	460	CYS	2.9
2	B	452	ASN	2.9
2	B	34	GLY	2.7
2	B	77	SER	2.6
2	B	35	SER	2.6
2	B	79	GLN	2.5
2	B	442	GLU	2.5
2	B	78	SER	2.4
2	B	453	GLY	2.4
2	B	461	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	447	ARG	2.3
2	B	441	ALA	2.3
2	B	48	ASN	2.3
2	B	9	GLY	2.3
1	A	452	PRO	2.2
2	B	449	ASN	2.2
1	A	1	LEU	2.1
2	B	28	ASP	2.1

## 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	NAG	B	3371	14/15	0.90	0.29	1.07	16,22,26,28	0
10	NAG	B	3321	14/15	0.92	0.30	-	18,21,28,35	0
11	MAN	B	3377	11/12	0.92	0.35	-	31,33,34,34	0
11	MAN	B	3375	11/12	0.96	0.20	-	20,23,26,27	0
10	NAG	B	3320	14/15	0.96	0.14	-	3,6,9,14	0
10	MAN	B	3324	11/12	0.78	0.41	-	54,56,57,57	0
11	MAN	B	3374	11/12	0.88	0.31	-	27,29,31,32	11
11	MAN	B	3376	11/12	0.92	0.20	-	17,19,20,21	0
11	NAG	B	3372	14/15	0.91	0.27	-	18,31,34,36	0
11	MAN	B	3373	11/12	0.92	0.27	-	30,35,36,37	0
10	MAN	B	3323	11/12	0.89	0.29	-	35,37,39,40	0
10	MAN	B	3322	11/12	0.84	0.33	-	38,43,50,54	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	B	1478	6/6	0.97	0.18	2.90	29,29,29,30	0
6	GOL	A	1461	6/6	0.93	0.19	0.34	15,16,17,17	0
9	180	B	1477	34/34	0.97	0.10	-1.60	2,2,2,2	0
7	CA	A	2004	1/1	0.96	0.06	-2.42	7,7,7,7	0
7	CA	A	2007	1/1	0.98	0.06	-2.89	3,3,3,3	0
7	CA	A	2005	1/1	0.95	0.05	-3.34	4,4,4,4	0
7	CA	A	2006	1/1	0.99	0.04	-3.46	12,12,12,12	0
5	MG	B	2001	1/1	0.98	0.04	-3.74	2,2,2,2	0
7	CA	B	2003	1/1	0.99	0.04	-6.93	2,2,2,2	0
8	NAG	A	3249	14/15	0.73	0.51	-	23,26,27,28	14
7	CA	B	2002	1/1	0.98	0.04	-	2,2,2,2	0
5	MG	A	1460	1/1	0.91	0.21	-	2,2,2,2	0
8	NAG	A	3015	14/15	0.76	0.49	-	40,44,46,47	0
8	NAG	B	3099	14/15	0.72	0.34	-	43,48,53,54	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.