



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 05:21 AM BST

PDB ID : 2VDL
Title : Re-refinement of Integrin AlphaIIbBeta3 Headpiece
Authors : Springer, T.A.; Zhu, J.; Xiao, T.
Deposited on : 2007-10-10
Resolution : 2.75 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

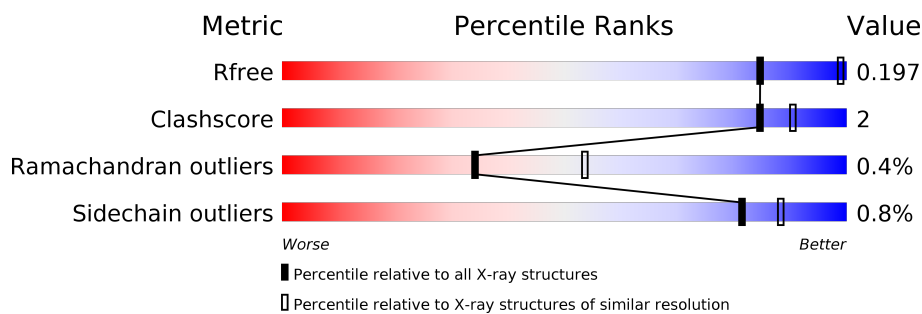
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	452	95% .
2	B	461	90% 8% .
3	H	221	94% 5% .
4	L	214	94% 6%
5	C	5	80% 20%
6	D	7	43% 57%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MAN	C	3	X	-	-	-
6	MAN	D	3	X	-	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 11800 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	8	0
			3520	2235	612	665	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	282	GLY	ALA	conflict	UNP P08514

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	456	Total	C	N	O	S	0	13	0
			3600	2249	614	704	33			

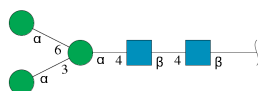
- Molecule 3 is a protein called MONOCLONAL ANTIBODY 10E5 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	219	Total	C	N	O	S	0	6	0
			1678	1065	270	337	6			

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

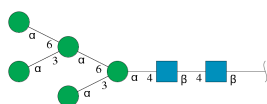
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	214	Total	C	N	O	S	0	7	0
			1663	1035	272	345	11			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



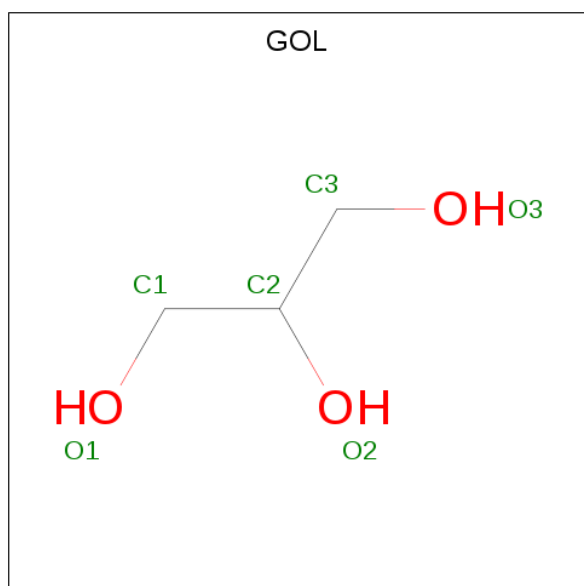
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	D	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

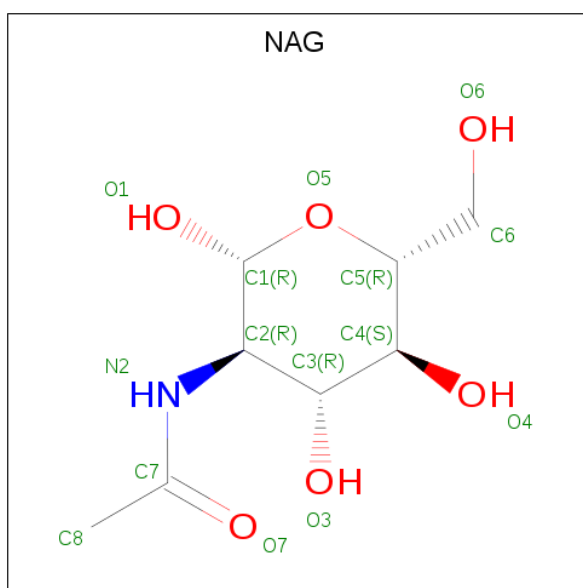


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

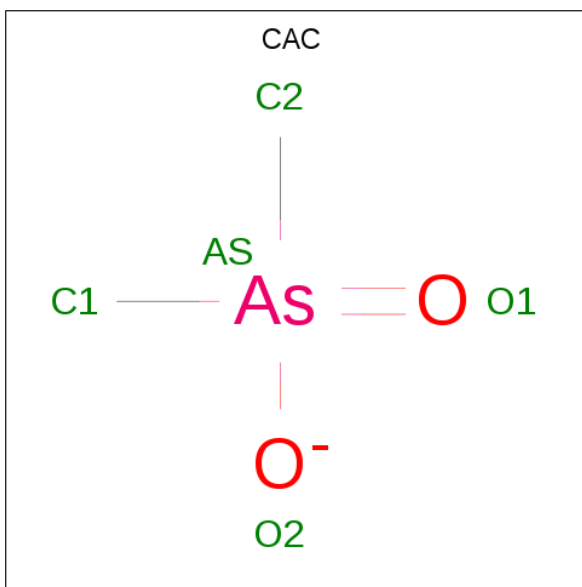
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	2	Total	Ca	0	0
			2	2		
8	A	4	Total	Ca	0	0
			4	4		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 10 is CACODYLATE ION (three-letter code: CAC) (formula: C₂H₆AsO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

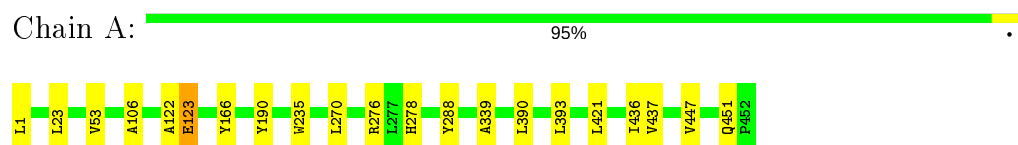
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	411	Total	O	0	0
			411	411		
12	B	250	Total	O	0	0
			250	250		
12	H	221	Total	O	0	0
			221	221		
12	L	247	Total	O	0	0
			247	247		

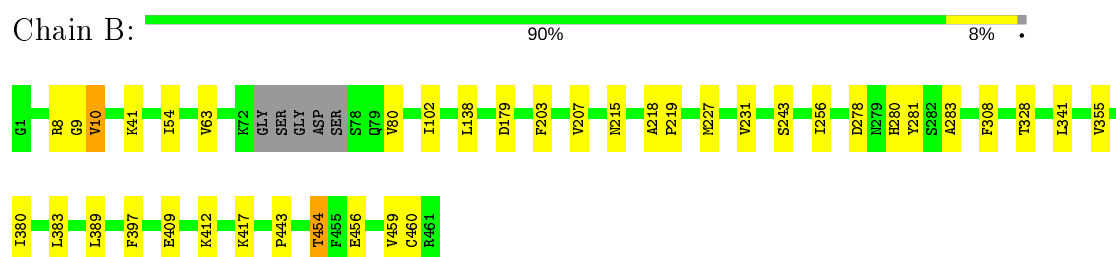
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

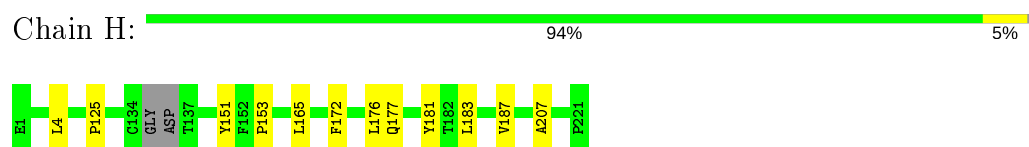
- Molecule 1: INTEGRIN ALPHA-IIB



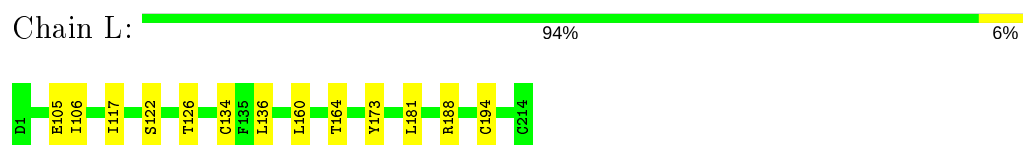
- Molecule 2: INTEGRIN BETA-3



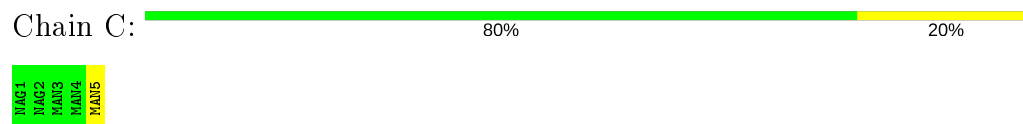
- Molecule 3: MONOCLONAL ANTIBODY 10E5 HEAVY CHAIN



- Molecule 4: MONOCLONAL ANTIBODY 10E5 LIGHT CHAIN



- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-6)-[α -D-mannopyranose-(1-3)] α -D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



MAN1	MAN2	MAN3	MAN4	MAN5	MAN6	MAN7
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4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	148.93Å 148.93Å 176.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.99 – 2.75 38.65 – 2.75	Depositor EDS
% Data completeness (in resolution range)	95.1 (42.99-2.75) 89.6 (38.65-2.75)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.50 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.144 , 0.191 0.150 , 0.197	Depositor DCC
R_{free} test set	2696 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11800	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, NAG, CA, CAC, 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	0/3629	0.52	0/4943
2	B	0.32	0/3688	0.49	0/4995
3	H	0.32	0/1730	0.51	0/2368
4	L	0.34	0/1719	0.53	0/2330
All	All	0.33	0/10766	0.51	0/14636

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3520	0	3361	11	0
2	B	3600	0	3548	20	0
3	H	1678	0	1634	8	0
4	L	1663	0	1581	11	0
5	C	61	0	52	0	0
6	D	83	0	70	0	0
7	A	6	0	8	0	0
7	B	6	0	8	0	0
8	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	2	0	0	0	0
9	A	28	0	26	0	0
9	B	14	0	13	0	0
10	B	5	0	0	1	0
11	B	1	0	0	0	0
12	A	411	0	0	2	0
12	B	250	0	0	2	0
12	H	221	0	0	1	0
12	L	247	0	0	2	0
All	All	11800	0	10301	49	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 (49) 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)
10:B:1462:CAC:C1	12:B:4099:HOH:O	2.23	0.86
3:H:177[A]:GLN:HB3	4:L:160:LEU:HD11	1.76	0.66
1:A:270:LEU:HD23	1:A:276:ARG:HA	1.80	0.62
2:B:138:LEU:HD23	2:B:341[A]:LEU:HD23	1.84	0.59
1:A:235:TRP:HZ2	1:A:270:LEU:HD11	1.72	0.55
2:B:456:GLU:O	2:B:459:VAL:HG12	2.06	0.55
3:H:177[A]:GLN:NE2	12:H:4196:HOH:O	2.38	0.53
2:B:355:VAL:HG23	2:B:389:LEU:HD22	1.91	0.52
1:A:235:TRP:CZ2	1:A:270:LEU:HD11	2.45	0.52
1:A:390:LEU:HD12	1:A:390:LEU:N	2.25	0.51
1:A:421:LEU:CD2	1:A:437:VAL:HG22	2.40	0.51
2:B:281:TYR:CE1	2:B:283:ALA:HB3	2.46	0.50
1:A:1:LEU:HB2	1:A:393:LEU:HD11	1.94	0.50
2:B:41:LYS:HG3	2:B:54:ILE:HG21	1.93	0.49
4:L:136:LEU:N	4:L:136:LEU:HD12	2.29	0.48
1:A:278[A]:HIS:CD2	1:A:339:ALA:HB1	2.48	0.48
2:B:278:ASP:CG	2:B:280[B]:HIS:HD1	2.17	0.48
1:A:451:GLN:NE2	12:A:4408:HOH:O	2.47	0.48
3:H:172:PHE:CD1	4:L:164:THR:HG23	2.49	0.47
4:L:122:SER:O	4:L:126:THR:HG23	2.16	0.46
2:B:102:ILE:HG22	2:B:397:PHE:HB2	1.97	0.46
2:B:63:VAL:HG23	2:B:63:VAL:O	2.15	0.46
3:H:165:LEU:CD2	3:H:187:VAL:HG21	2.46	0.46
3:H:4:LEU:N	3:H:4:LEU:HD12	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:308:PHE:CE2	2:B:328:THR:HG21	2.50	0.45
4:L:117:ILE:HG13	4:L:134[B]:CYS:SG	2.57	0.45
3:H:176:LEU:HD13	3:H:181:TYR:CE1	2.51	0.45
2:B:203:PHE:O	2:B:207:VAL:HG23	2.17	0.45
2:B:8:ARG:O	2:B:10:VAL:N	2.51	0.44
3:H:125:PRO:HB3	3:H:151:TYR:HB3	2.00	0.44
4:L:181:LEU:N	4:L:181:LEU:HD23	2.33	0.44
2:B:218:ALA:HB3	2:B:219:PRO:HD3	2.00	0.43
1:A:436:ILE:HG22	1:A:447:VAL:HG22	1.99	0.43
2:B:459:VAL:HG22	2:B:460:CYS:O	2.19	0.43
2:B:278:ASP:OD2	2:B:280[B]:HIS:ND1	2.51	0.43
4:L:105:GLU:HG3	4:L:173:TYR:OH	2.19	0.43
1:A:122:ALA:O	1:A:123:GLU:HB2	2.18	0.42
2:B:227:MET:O	2:B:231:VAL:HG22	2.19	0.42
2:B:380:ILE:HG21	2:B:383:LEU:HD22	2.01	0.42
2:B:417:LYS:NZ	12:B:4224:HOH:O	2.53	0.42
1:A:53:VAL:HG21	1:A:106:ALA:CB	2.49	0.42
4:L:117:ILE:HA	4:L:134[B]:CYS:SG	2.60	0.42
2:B:443:PRO:HA	2:B:454:THR:HG22	2.02	0.42
2:B:409:GLU:HB2	2:B:412[B]:LYS:HZ2	1.84	0.41
4:L:106:ILE:HD12	12:L:4203:HOH:O	2.21	0.41
12:A:4301:HOH:O	2:B:256:ILE:HD12	2.21	0.41
4:L:188[B]:ARG:NH2	12:L:4224:HOH:O	2.54	0.40
3:H:153:PRO:HD2	3:H:207:ALA:CB	2.52	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	457/452 (101%)	445 (97%)	11 (2%)	1 (0%)	47 69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	463/461 (100%)	442 (96%)	17 (4%)	4 (1%)	17	31
3	H	218/221 (99%)	213 (98%)	5 (2%)	0	100	100
4	L	218/214 (102%)	211 (97%)	7 (3%)	0	100	100
All	All	1356/1348 (101%)	1311 (97%)	40 (3%)	5 (0%)	34	53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
2	B	9	GLY
2	B	80	VAL
2	B	454	THR
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	367/360 (102%)	363 (99%)	4 (1%)	73	84
2	B	417/409 (102%)	414 (99%)	3 (1%)	84	89
3	H	192/190 (101%)	191 (100%)	1 (0%)	88	92
4	L	194/188 (103%)	192 (99%)	2 (1%)	76	85
All	All	1170/1147 (102%)	1160 (99%)	10 (1%)	81	87

All (10) 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	179	ASP
2	B	215	ASN

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Mol	Chain	Res	Type
2	B	243	SER
3	H	183	LEU
4	L	194[A]	CYS
4	L	194[B]	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	199	GLN
2	B	316	ASN
2	B	342	GLN
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 monosaccharides 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	$\# Z > 2$
5	NAG	C	1	2,5	14,14,15	0.60	0	17,19,21	0.77	0
5	NAG	C	2	5	14,14,15	0.72	0	17,19,21	0.92	0
5	MAN	C	3	5	11,11,12	0.64	0	15,15,17	0.62	0
5	MAN	C	4	5	11,11,12	0.53	0	15,15,17	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	C	5	5	11,11,12	0.58	0	15,15,17	1.51	2 (13%)
6	NAG	D	1	2,6	14,14,15	0.71	0	17,19,21	1.01	1 (5%)
6	NAG	D	2	6	14,14,15	0.50	0	17,19,21	0.97	0
6	MAN	D	3	6	11,11,12	0.57	0	15,15,17	0.91	1 (6%)
6	MAN	D	4	6	11,11,12	0.71	0	15,15,17	1.04	1 (6%)
6	MAN	D	5	6	11,11,12	0.57	0	15,15,17	0.96	0
6	MAN	D	6	6	11,11,12	0.59	0	15,15,17	0.74	0
6	MAN	D	7	6	11,11,12	0.61	0	15,15,17	1.14	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
5	NAG	C	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	C	2	5	-	1/6/23/26	0/1/1/1
5	MAN	C	3	5	1/1/4/5	0/2/19/22	0/1/1/1
5	MAN	C	4	5	-	0/2/19/22	0/1/1/1
5	MAN	C	5	5	-	0/2/19/22	0/1/1/1
6	NAG	D	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	D	2	6	-	0/6/23/26	0/1/1/1
6	MAN	D	3	6	1/1/4/5	2/2/19/22	0/1/1/1
6	MAN	D	4	6	-	0/2/19/22	0/1/1/1
6	MAN	D	5	6	-	0/2/19/22	0/1/1/1
6	MAN	D	6	6	-	2/2/19/22	0/1/1/1
6	MAN	D	7	6	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	5	MAN	C1-O5-C5	3.70	117.21	112.19
5	C	5	MAN	C1-C2-C3	3.35	113.78	109.67
6	D	4	MAN	C1-O5-C5	3.00	116.26	112.19
6	D	7	MAN	C3-C4-C5	2.71	115.06	110.24
6	D	1	NAG	O5-C1-C2	-2.33	107.61	111.29
6	D	3	MAN	O5-C5-C6	2.09	110.48	107.20

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	3	MAN	C1
6	D	3	MAN	C1

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	3	MAN	O5-C5-C6-O6
6	D	6	MAN	C4-C5-C6-O6
6	D	6	MAN	O5-C5-C6-O6
6	D	3	MAN	C4-C5-C6-O6
5	C	2	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 7 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	$\# Z > 2$
10	CAC	B	1462	11	0,4,4	0.00	-	0,6,6	0.00	-
9	NAG	B	3099	2	14,14,15	0.58	0	17,19,21	1.01	0
7	GOL	A	1453	-	5,5,5	0.42	0	5,5,5	0.17	0
9	NAG	A	3249	1	14,14,15	0.50	0	17,19,21	1.21	2 (11%)
9	NAG	A	3015	1	14,14,15	0.48	0	17,19,21	1.03	0
7	GOL	B	1463	8	5,5,5	0.37	0	5,5,5	0.21	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
7	GOL	A	1453	-	-	2/4/4/4	-
9	NAG	B	3099	2	-	2/6/23/26	0/1/1/1
9	NAG	A	3249	1	-	2/6/23/26	0/1/1/1
9	NAG	A	3015	1	-	0/6/23/26	0/1/1/1
7	GOL	B	1463	8	-	0/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	3249	NAG	O5-C5-C6	2.76	111.53	107.20
9	A	3249	NAG	C1-O5-C5	2.22	115.20	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1453	GOL	O1-C1-C2-O2
7	A	1453	GOL	O1-C1-C2-C3
9	A	3249	NAG	O5-C5-C6-O6
9	A	3249	NAG	C4-C5-C6-O6
9	B	3099	NAG	O5-C5-C6-O6
9	B	3099	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	1462	CAC	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.