



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:45 PM GMT

PDB ID : 4MMZ
Title : Integrin AlphaVBeta3 ectodomain bound to an antagonistic tenth domain of Fibronectin
Authors : van Agthoven, J.; Xiong, J.; Arnaout, M.A.
Deposited on : 2013-09-09
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at 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.

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

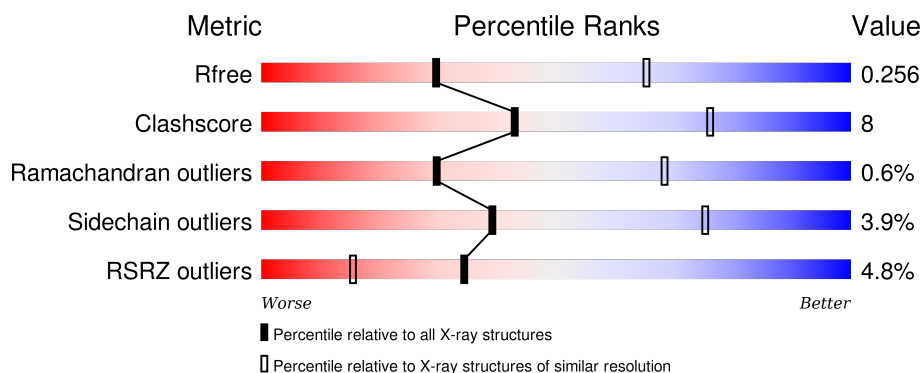
1 Overall quality at a glance

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 ≥ 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	959	<div> <div>2%</div> <div>76%</div> <div>20%</div> <div>• •</div> </div>
2	B	692	<div> <div>6%</div> <div>76%</div> <div>21%</div> <div>•</div> </div>
3	C	98	<div> <div>18%</div> <div>68%</div> <div>21%</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
9	GOL	A	1024	-	-	-	X
9	GOL	C	1601	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 13501 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-V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	920	Total	C	N	O	S	0	0	0
			7163	4535	1216	1377	35			

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	690	Total	C	N	O	S	0	0	0
			5294	3250	904	1070	70			

- Molecule 3 is a protein called Fibronectin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	91	Total	C	N	O	0	0	0
			690	439	112	139			

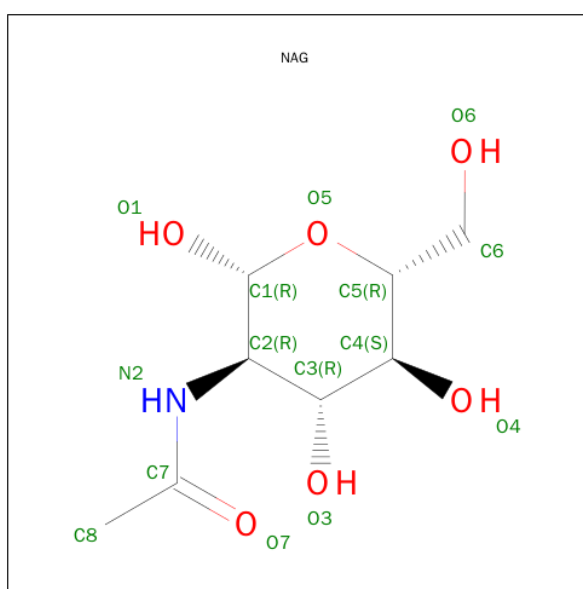
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1492	PRO	GLY	ENGINEERED MUTATION	UNP P02751
C	1496	TRP	SER	ENGINEERED MUTATION	UNP P02751
C	1497	ASN	PRO	ENGINEERED MUTATION	UNP P02751
C	1498	GLU	ALA	ENGINEERED MUTATION	UNP P02751
C	1499	GLY	SER	ENGINEERED MUTATION	UNP P02751
C	1510	GLY	-	EXPRESSION TAG	UNP P02751
C	1511	LYS	-	EXPRESSION TAG	UNP P02751
C	1512	LYS	-	EXPRESSION TAG	UNP P02751
C	1513	GLY	-	EXPRESSION TAG	UNP P02751
C	1514	LYS	-	EXPRESSION TAG	UNP P02751

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	6	Total	C	N	O	0	0
			72	40	2	30		

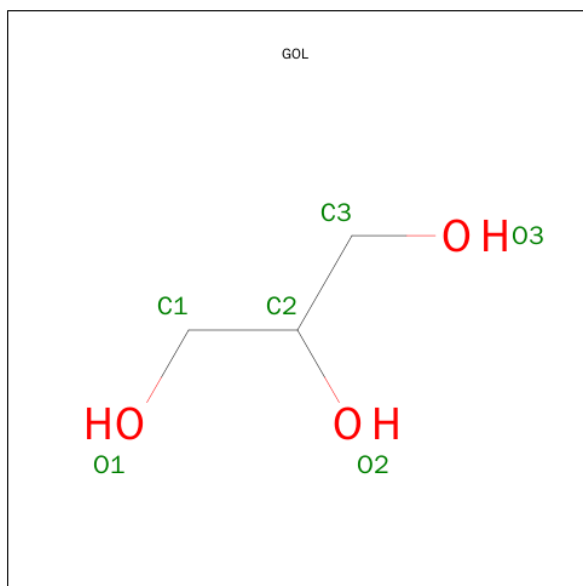
- Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	3	Total	Mn	0	0
			3	3		
7	A	5	Total	Mn	0	0
			5	5		

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Na	0	0
			1	1		
8	A	1	Total	Na	0	0
			1	1		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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

- Molecule 10 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	2	Total	Cl	0	0
			2	2		

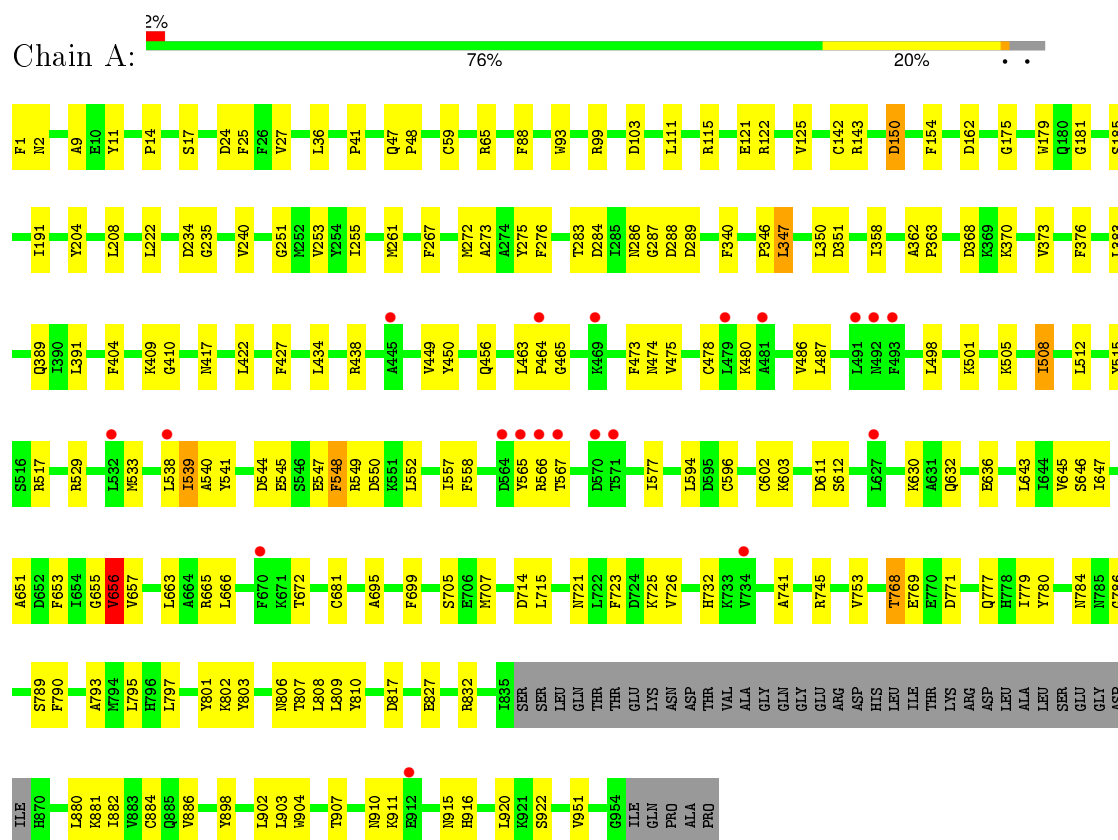
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	2	Total	O	0	0
			2	2		
12	B	2	Total	O	0	0
			2	2		
12	C	5	Total	O	0	0
			5	5		

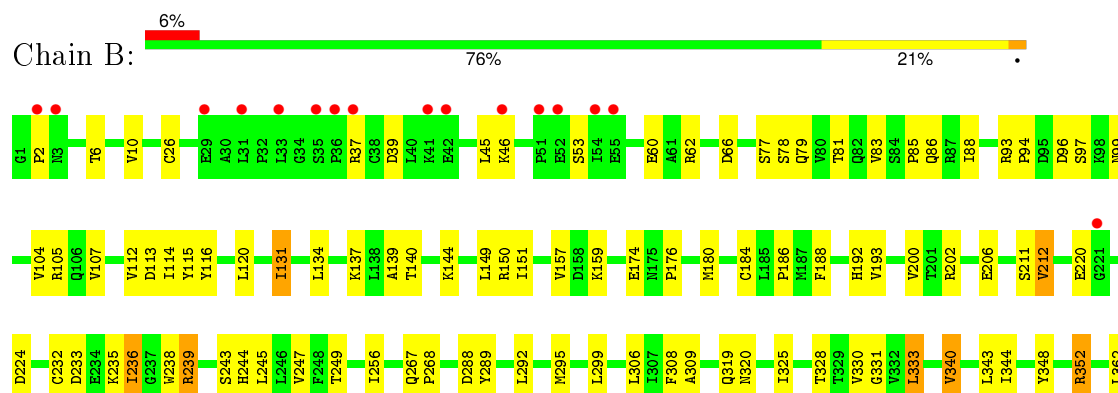
3 Residue-property plots

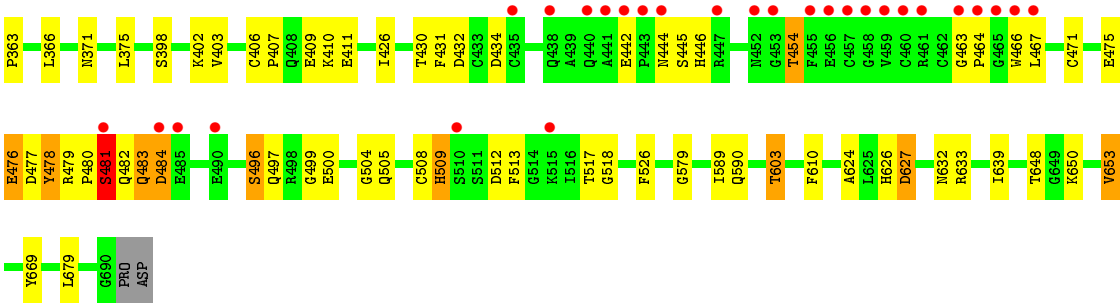
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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-V

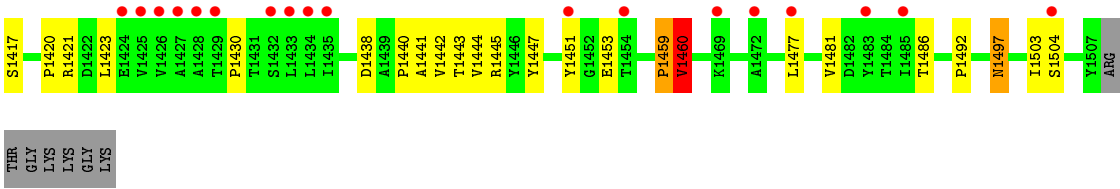


• Molecule 2: Integrin beta-3





● Molecule 3: Fibronectin



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	129.79Å 129.79Å 307.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.48 – 3.10 42.48 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.48-3.10) 99.9 (42.48-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.12Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.4_1496)	Depositor
R, R_{free}	0.203 , 0.256 0.203 , 0.256	Depositor DCC
R_{free} test set	2704 reflections (4.90%)	DCC
Wilson B-factor (Å ²)	94.8	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 64.2	EDS
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 55192 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13501	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, BMA, NAG, CL, NA, MN, 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	0.24	0/7319	0.46	0/9922
2	B	0.24	0/5390	0.48	1/7289 (0.0%)
3	C	0.24	0/708	0.51	0/974
All	All	0.24	0/13417	0.47	1/18185 (0.0%)

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
1	A	0	1
2	B	0	3
3	C	0	1
All	All	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	239	ARG	CB-CA-C	5.28	120.96	110.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	539	ILE	Peptide
2	B	476	GLU	Peptide
2	B	481	SER	Peptide

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Mol	Chain	Res	Type	Group
2	B	632	ASN	Peptide
3	C	1451	TYR	Peptide

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	7163	0	6982	112	0
2	B	5294	0	5025	93	0
3	C	690	0	675	11	0
4	A	84	0	75	2	0
4	B	28	0	25	0	0
5	A	70	0	65	1	0
5	B	28	0	26	1	0
6	A	72	0	61	1	0
7	A	5	0	0	0	0
7	B	3	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	6	0	8	0	0
9	C	6	0	8	0	0
10	B	39	0	34	1	0
11	B	2	0	0	0	0
12	A	2	0	0	0	0
12	B	2	0	0	0	0
12	C	5	0	0	1	0
All	All	13501	0	12984	216	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 8.

The worst 5 of 216 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:114:ILE:HG22	2:B:245:LEU:HB2	1.62	0.79
2:B:366:LEU:HB3	2:B:403:VAL:HG12	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ALA:HB3	1:A:434:LEU:HB3	1.70	0.73
1:A:450:TYR:HB2	1:A:474:ASN:HB2	1.70	0.72
1:A:548:PHE:HB2	1:A:550:ASP:H	1.57	0.69

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	916/959 (96%)	836 (91%)	76 (8%)	4 (0%)	39	75
2	B	688/692 (99%)	603 (88%)	83 (12%)	2 (0%)	46	80
3	C	89/98 (91%)	74 (83%)	10 (11%)	5 (6%)	2	13
All	All	1693/1749 (97%)	1513 (89%)	169 (10%)	11 (1%)	30	68

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	1459	PRO
3	C	1460	VAL
3	C	1453	GLU
1	A	552	LEU
1	A	565	TYR

5.3.2 Protein sidechains [i](#)

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	780/813 (96%)	756 (97%)	24 (3%)	47	80
2	B	612/614 (100%)	582 (95%)	30 (5%)	31	68
3	C	77/82 (94%)	74 (96%)	3 (4%)	39	75
All	All	1469/1509 (97%)	1412 (96%)	57 (4%)	39	75

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	45	LEU
2	B	211	SER
2	B	650	LYS
2	B	46	LYS
2	B	131	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	1461	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 ⓘ

17 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
4	NAG	A	1001	1,4	14,14,15	0.34	0	15,19,21	0.23	0
4	NAG	A	1002	4	14,14,15	0.26	0	15,19,21	0.27	0
6	NAG	A	1004	1,6	14,14,15	0.44	0	15,19,21	0.29	0
6	NAG	A	1005	6	14,14,15	0.24	0	15,19,21	0.35	0
6	BMA	A	1006	6	11,11,12	0.69	0	14,15,17	0.88	1 (7%)
6	MAN	A	1007	6	11,11,12	0.74	0	14,15,17	1.03	2 (14%)
6	BMA	A	1008	6	11,11,12	1.22	1 (9%)	14,15,17	1.10	0
6	MAN	A	1009	6	11,11,12	1.05	1 (9%)	14,15,17	0.94	1 (7%)
4	NAG	A	1010	1,4	14,14,15	0.51	0	15,19,21	1.34	1 (6%)
4	NAG	A	1011	4	14,14,15	0.28	0	15,19,21	0.29	0
4	NAG	A	1014	1,4	14,14,15	0.32	0	15,19,21	0.63	0
4	NAG	A	1015	4	14,14,15	0.42	0	15,19,21	0.67	1 (6%)
4	NAG	B	703	2,4	14,14,15	0.31	0	15,19,21	0.36	0
4	NAG	B	704	4	14,14,15	0.64	0	15,19,21	0.80	1 (6%)
10	NAG	B	705	10,2	14,14,15	0.27	0	15,19,21	0.34	0
10	NAG	B	706	10	14,14,15	0.61	1 (7%)	15,19,21	1.42	1 (6%)
10	BMA	B	707	10	11,11,12	0.89	0	14,15,17	1.18	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
4	NAG	A	1001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1002	4	-	0/6/23/26	0/1/1/1
6	NAG	A	1004	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1005	6	-	0/6/23/26	0/1/1/1
6	BMA	A	1006	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1007	6	-	0/2/19/22	0/1/1/1
6	BMA	A	1008	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1009	6	-	0/2/19/22	0/1/1/1
4	NAG	A	1010	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1011	4	-	0/6/23/26	0/1/1/1
4	NAG	A	1014	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1015	4	-	0/6/23/26	0/1/1/1
4	NAG	B	703	2,4	-	0/6/23/26	0/1/1/1
4	NAG	B	704	4	-	0/6/23/26	0/1/1/1
10	NAG	B	705	10,2	-	0/6/23/26	0/1/1/1
10	NAG	B	706	10	-	0/6/23/26	0/1/1/1
10	BMA	B	707	10	-	0/2/19/22	1/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1009	MAN	O5-C1	-2.39	1.39	1.43
10	B	706	NAG	C1-C2	2.03	1.55	1.52
6	A	1008	BMA	C4-C5	2.43	1.58	1.53

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1007	MAN	O2-C2-C3	-2.34	105.42	110.12
6	A	1009	MAN	O2-C2-C3	-2.20	105.69	110.12
6	A	1007	MAN	C1-O5-C5	2.15	114.97	112.25
6	A	1006	BMA	C1-O5-C5	2.30	115.17	112.25
4	A	1015	NAG	C1-O5-C5	2.55	115.49	112.25

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	707	BMA	C1-C2-C3-C4-C5-O5

6 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1008	BMA	1	0
6	A	1009	MAN	1	0
4	A	1010	NAG	1	0
4	A	1014	NAG	1	0
4	A	1015	NAG	1	0
10	B	706	NAG	1	0

5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 12 are monoatomic - leaving 9 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
5	NAG	A	1003	1	14,14,15	0.73	1 (7%)	15,19,21	1.11	1 (6%)
5	NAG	A	1012	1	14,14,15	0.46	0	15,19,21	1.28	1 (6%)
5	NAG	A	1013	1	14,14,15	0.24	0	15,19,21	0.38	0
5	NAG	A	1016	1	14,14,15	0.25	0	15,19,21	0.31	0
5	NAG	A	1017	1	14,14,15	0.26	0	15,19,21	0.39	0
9	GOL	A	1024	-	5,5,5	0.35	0	5,5,5	0.26	0
5	NAG	B	701	2	14,14,15	0.41	0	15,19,21	0.64	1 (6%)
5	NAG	B	702	2	14,14,15	0.26	0	15,19,21	0.26	0
9	GOL	C	1601	-	5,5,5	0.34	0	5,5,5	0.22	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
5	NAG	A	1003	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1012	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1013	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1016	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1017	1	-	0/6/23/26	0/1/1/1
9	GOL	A	1024	-	-	0/4/4/4	0/0/0/0
5	NAG	B	701	2	-	0/6/23/26	0/1/1/1
5	NAG	B	702	2	-	0/6/23/26	0/1/1/1
9	GOL	C	1601	-	-	0/4/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1003	NAG	O5-C1	2.59	1.48	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	701	NAG	C1-O5-C5	2.40	115.30	112.25
5	A	1003	NAG	C1-O5-C5	4.17	117.54	112.25
5	A	1012	NAG	C2-N2-C7	4.70	129.08	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1012	NAG	1	0
5	B	701	NAG	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q < 0.9
1	A	920/959 (95%)	-0.01	20 (2%) 65 42	56, 101, 157, 192	0
2	B	690/692 (99%)	0.18	44 (6%) 23 9	61, 115, 215, 262	2 (0%)
3	C	91/98 (92%)	1.17	18 (19%) 1 0	76, 162, 235, 280	0
All	All	1701/1749 (97%)	0.13	82 (4%) 34 15	56, 109, 197, 280	2 (0%)

The worst 5 of 82 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	510	SER	9.9
3	C	1426	VAL	6.6
3	C	1425	VAL	6.3
3	C	1428	ALA	5.7
3	C	1432	SER	5.6

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, 95th 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 ²)	Q < 0.9
4	NAG	B	703	14/15	0.96	0.16	-0.47	80,115,125,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
10	NAG	B	705	14/15	0.94	0.18	-0.80	75,99,122,124	0
6	NAG	A	1004	14/15	0.97	0.19	-0.96	53,69,117,118	0
4	NAG	A	1001	14/15	0.95	0.12	-1.13	60,95,121,133	0
4	NAG	A	1014	14/15	0.83	0.16	-1.20	101,119,137,163	0
6	MAN	A	1009	11/12	0.85	0.21	-	153,158,164,166	0
6	BMA	A	1006	11/12	0.95	0.13	-	107,123,142,145	0
4	NAG	A	1011	14/15	0.87	0.33	-	124,160,171,183	0
4	NAG	A	1015	14/15	0.77	0.20	-	132,157,176,176	0
4	NAG	A	1002	14/15	0.91	0.17	-	116,140,150,164	0
6	NAG	A	1005	14/15	0.98	0.18	-	46,73,97,115	0
10	NAG	B	706	14/15	0.92	0.22	-	127,139,159,163	0
6	BMA	A	1008	11/12	0.82	0.18	-	135,149,158,159	0
4	NAG	B	704	14/15	0.87	0.23	-	161,172,177,178	0
10	BMA	B	707	11/12	0.84	0.14	-	115,142,158,158	0
4	NAG	A	1010	14/15	0.86	0.18	-	98,132,143,154	0
6	MAN	A	1007	11/12	0.87	0.22	-	137,145,156,162	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, 95th 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 ²)	Q<0.9
9	GOL	C	1601	6/6	0.83	0.71	12.30	131,136,144,145	0
9	GOL	A	1024	6/6	0.69	0.67	9.66	139,143,149,151	0
5	NAG	B	702	14/15	0.89	0.27	0.32	104,156,161,165	0
7	MN	A	1019	1/1	0.66	0.17	0.30	181,181,181,181	0
7	MN	B	709	1/1	0.96	0.19	0.20	99,99,99,99	0
7	MN	A	1022	1/1	0.96	0.13	0.07	131,131,131,131	0
8	NA	A	1023	1/1	0.99	0.22	-0.20	89,89,89,89	0
7	MN	A	1020	1/1	0.97	0.14	-0.54	132,132,132,132	0
7	MN	A	1021	1/1	0.99	0.18	-0.64	175,175,175,175	0
7	MN	B	708	1/1	0.98	0.22	-0.70	73,73,73,73	0
7	MN	A	1018	1/1	0.92	0.10	-0.88	132,132,132,132	0
5	NAG	A	1012	14/15	0.89	0.12	-1.42	116,141,155,157	0
7	MN	B	710	1/1	0.97	0.23	-2.08	103,103,103,103	0
5	NAG	A	1016	14/15	0.87	0.15	-	103,140,146,150	0
5	NAG	A	1017	14/15	0.91	0.23	-	82,119,149,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	NA	B	711	1/1	0.96	0.13	-	115,115,115,115	0
5	NAG	A	1013	14/15	0.84	0.37	-	129,154,161,171	0
11	CL	B	712	1/1	0.86	0.12	-	123,123,123,123	0
5	NAG	A	1003	14/15	0.90	0.16	-	84,112,128,134	0
11	CL	B	713	1/1	0.84	0.17	-	142,142,142,142	0
5	NAG	B	701	14/15	0.77	0.28	-	141,165,182,187	0

6.5 Other polymers [i](#)

There are no such residues in this entry.