



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2016 – 07:26 AM EDT

PDB ID : 5F7N
Title : Blood group antigen binding adhesin BabA of Helicobacter pylori strain 17875
in complex with blood group A Lewis b pentasaccharide
Authors : Moonens, K.; Gideonsson, P.; Subedi, S.; Romao, E.; Oscarson, S.; Muylder-
mans, S.; Boren, T.; Remaut, H.
Deposited on : 2015-12-08
Resolution : 2.28 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
<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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027674
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) : rb-20027674

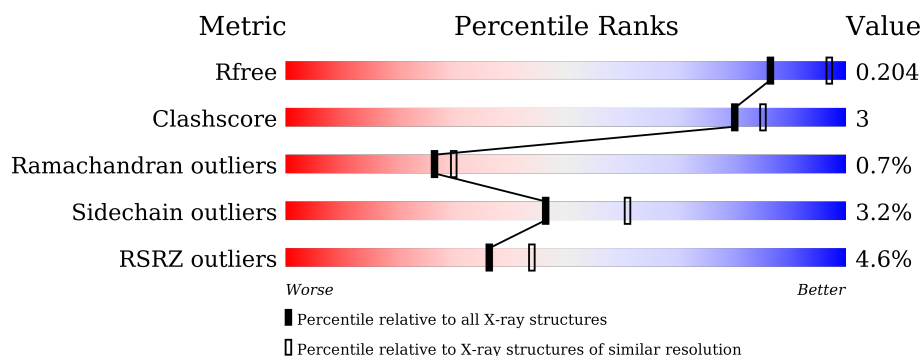
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	5193 (2.30-2.26)
Clashscore	102246	5929 (2.30-2.26)
Ramachandran outliers	100387	5851 (2.30-2.26)
Sidechain outliers	100360	5850 (2.30-2.26)
RSRZ outliers	91569	5204 (2.30-2.26)

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	466	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>7%</div> <div>11%</div> </div> </div>
1	B	466	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>7%</div> <div>10%</div> </div> </div>
2	C	120	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>6%</div> </div> </div>
2	D	120	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div></div> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	501	-	-	-	X
5	A2G	A	503	-	-	-	X
5	A2G	B	503	-	-	-	X
6	FUC	B	504	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8323 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 Adhesin binding fucosylated histo-blood group antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3098	1910	535	640	13			
1	B	420	Total	C	N	O	S	0	1	0
			3132	1930	540	649	13			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ALA	-	expression tag	UNP O52269
A	4	SER	-	expression tag	UNP O52269
A	5	TRP	-	expression tag	UNP O52269
A	6	SER	-	expression tag	UNP O52269
A	7	HIS	-	expression tag	UNP O52269
A	8	PRO	-	expression tag	UNP O52269
A	9	GLN	-	expression tag	UNP O52269
A	10	PHE	-	expression tag	UNP O52269
A	11	GLU	-	expression tag	UNP O52269
A	12	LYS	-	expression tag	UNP O52269
A	13	SER	-	expression tag	UNP O52269
A	14	GLY	-	expression tag	UNP O52269
A	15	GLY	-	expression tag	UNP O52269
A	16	GLY	-	expression tag	UNP O52269
A	17	GLY	-	expression tag	UNP O52269
A	18	GLY	-	expression tag	UNP O52269
A	19	LEU	-	expression tag	UNP O52269
A	20	VAL	-	expression tag	UNP O52269
A	21	PRO	-	expression tag	UNP O52269
A	22	ARG	-	expression tag	UNP O52269
A	23	GLY	-	expression tag	UNP O52269
A	24	SER	-	expression tag	UNP O52269
A	461	GLY	-	expression tag	UNP O52269
A	462	SER	-	expression tag	UNP O52269
A	463	HIS	-	expression tag	UNP O52269

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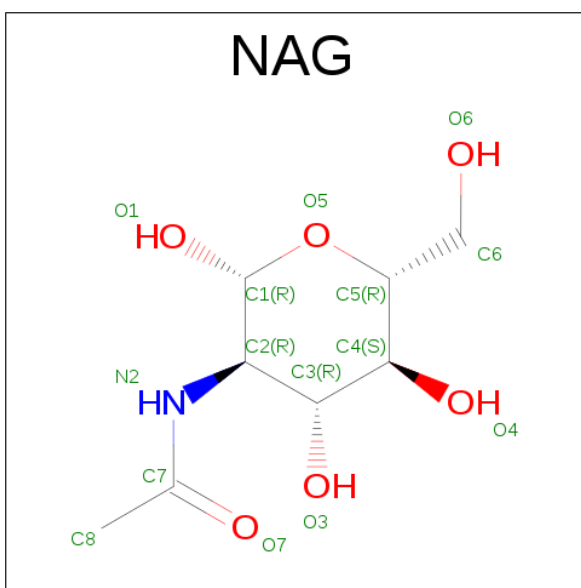
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Chain	Residue	Modelled	Actual	Comment	Reference
A	464	HIS	-	expression tag	UNP O52269
A	465	HIS	-	expression tag	UNP O52269
A	466	HIS	-	expression tag	UNP O52269
A	467	HIS	-	expression tag	UNP O52269
A	468	HIS	-	expression tag	UNP O52269
B	3	ALA	-	expression tag	UNP O52269
B	4	SER	-	expression tag	UNP O52269
B	5	TRP	-	expression tag	UNP O52269
B	6	SER	-	expression tag	UNP O52269
B	7	HIS	-	expression tag	UNP O52269
B	8	PRO	-	expression tag	UNP O52269
B	9	GLN	-	expression tag	UNP O52269
B	10	PHE	-	expression tag	UNP O52269
B	11	GLU	-	expression tag	UNP O52269
B	12	LYS	-	expression tag	UNP O52269
B	13	SER	-	expression tag	UNP O52269
B	14	GLY	-	expression tag	UNP O52269
B	15	GLY	-	expression tag	UNP O52269
B	16	GLY	-	expression tag	UNP O52269
B	17	GLY	-	expression tag	UNP O52269
B	18	GLY	-	expression tag	UNP O52269
B	19	LEU	-	expression tag	UNP O52269
B	20	VAL	-	expression tag	UNP O52269
B	21	PRO	-	expression tag	UNP O52269
B	22	ARG	-	expression tag	UNP O52269
B	23	GLY	-	expression tag	UNP O52269
B	24	SER	-	expression tag	UNP O52269
B	461	GLY	-	expression tag	UNP O52269
B	462	SER	-	expression tag	UNP O52269
B	463	HIS	-	expression tag	UNP O52269
B	464	HIS	-	expression tag	UNP O52269
B	465	HIS	-	expression tag	UNP O52269
B	466	HIS	-	expression tag	UNP O52269
B	467	HIS	-	expression tag	UNP O52269
B	468	HIS	-	expression tag	UNP O52269

- Molecule 2 is a protein called Nanobody Nb-ER19.

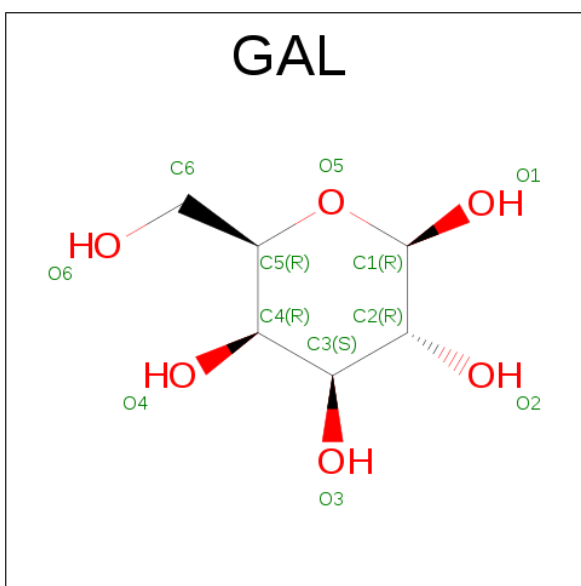
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	113	Total	C	N	O	S	0	0	0
			863	540	155	163	5			
2	D	115	Total	C	N	O	S	0	0	0
			883	552	161	165	5			

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	8	1	6		
3	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 4 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



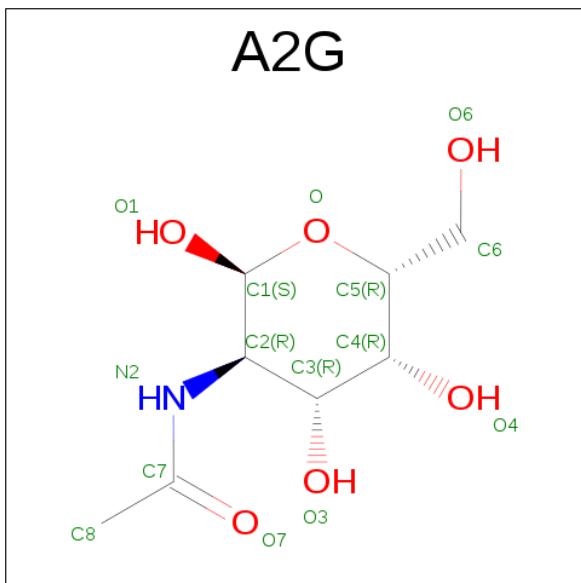
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		

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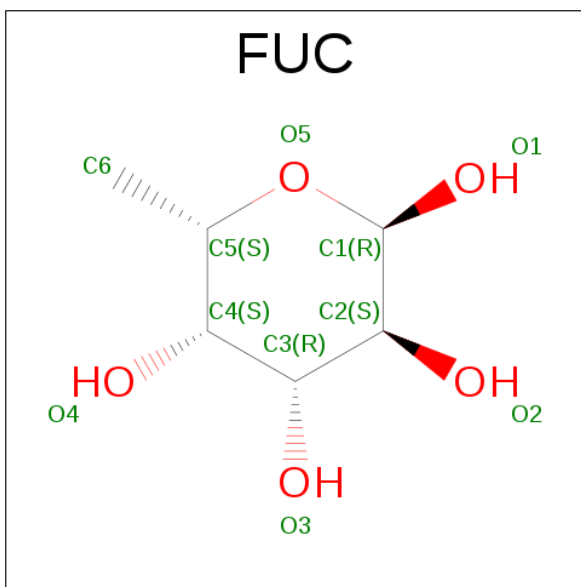
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is N-ACETYL-2-DEOXY-2-AMINO-GALACTOSE (three-letter code: A2G) (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	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		
6	A	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			10	6	4		

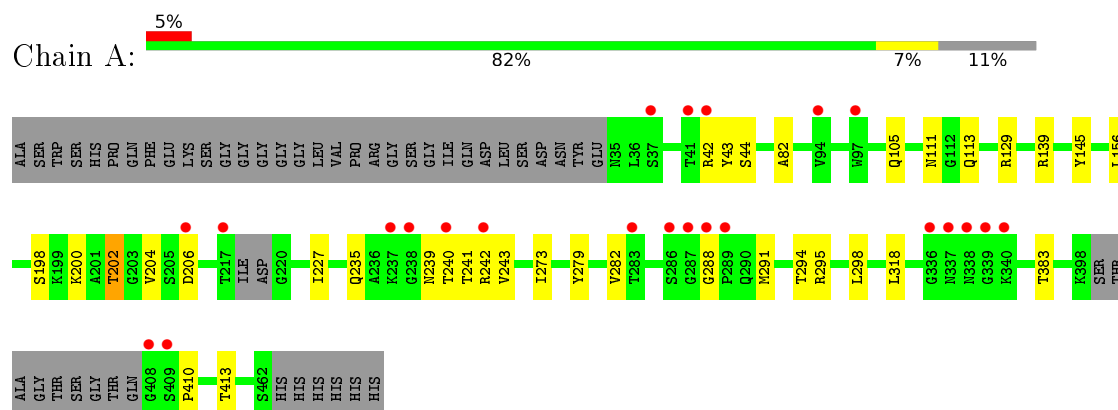
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	81	Total	O	0	0
			81	81		
7	B	71	Total	O	0	0
			71	71		
7	C	21	Total	O	0	0
			21	21		
7	D	54	Total	O	0	0
			54	54		

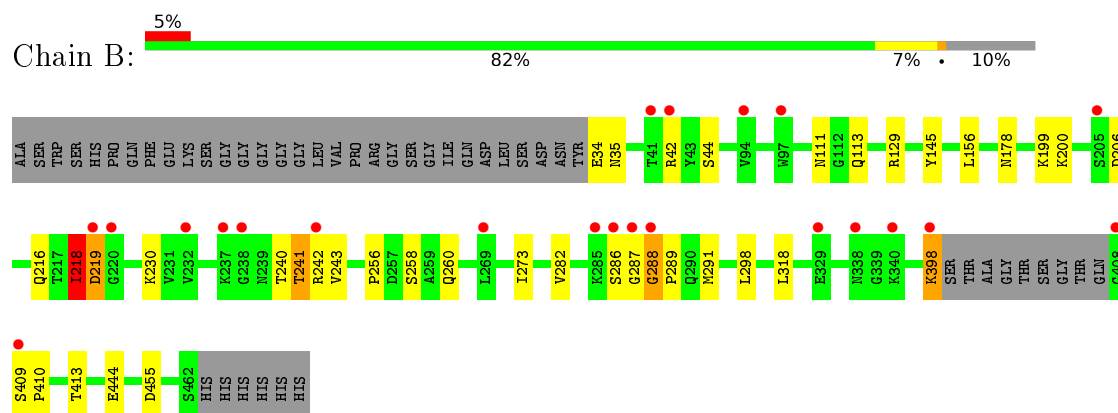
3 Residue-property plots

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.

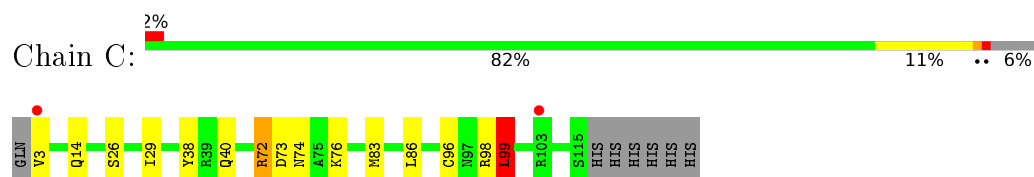
- Molecule 1: Adhesin binding fucosylated histo-blood group antigen



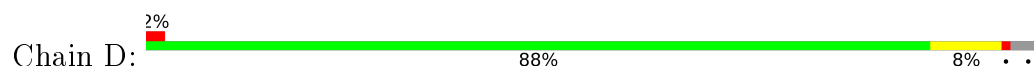
- Molecule 1: Adhesin binding fucosylated histo-blood group antigen

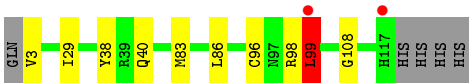


- Molecule 2: Nanobody Nb-ER19



- Molecule 2: Nanobody Nb-ER19





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.85Å 131.95Å 123.81Å 90.00° 94.81° 90.00°	Depositor
Resolution (Å)	33.20 – 2.28 33.22 – 2.28	Depositor EDS
% Data completeness (in resolution range)	98.4 (33.20-2.28) 98.5 (33.22-2.28)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.171 , 0.197 0.183 , 0.204	Depositor DCC
R_{free} test set	3651 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	47.4	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8323	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, GAL, NAG, A2G

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	0.91	1/3143 (0.0%)	0.88	1/4270 (0.0%)
1	B	0.88	1/3178 (0.0%)	0.85	2/4319 (0.0%)
2	C	0.99	0/882	1.01	4/1195 (0.3%)
2	D	1.08	1/904 (0.1%)	0.99	2/1225 (0.2%)
All	All	0.93	3/8107 (0.0%)	0.90	9/11009 (0.1%)

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	B	0	1
2	D	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	444	GLU	CG-CD	5.70	1.60	1.51
1	A	105	GLN	CG-CD	5.43	1.63	1.51
2	D	108	GLY	C-O	-5.27	1.15	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	72	ARG	NE-CZ-NH2	-9.79	115.40	120.30
2	C	72	ARG	NE-CZ-NH1	9.15	124.87	120.30
2	D	98	ARG	NE-CZ-NH1	6.26	123.43	120.30
2	C	99	LEU	CA-CB-CG	5.36	127.62	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	42	ARG	NE-CZ-NH1	5.25	122.93	120.30
2	C	98	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	B	318	LEU	CA-CB-CG	5.11	127.05	115.30
2	D	99	LEU	CA-CB-CG	5.05	126.92	115.30
1	A	139	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	286	SER	Peptide
2	D	3	VAL	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	3098	0	3028	19	0
1	B	3132	0	3057	26	0
2	C	863	0	845	7	0
2	D	883	0	859	2	0
3	A	15	0	13	0	0
3	B	15	0	13	0	0
4	A	11	0	8	0	0
4	B	11	0	8	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
6	A	20	0	20	0	0
6	B	20	0	20	0	0
7	A	81	0	0	1	0
7	B	71	0	0	1	0
7	C	21	0	0	1	0
7	D	54	0	0	0	0
All	All	8323	0	7897	54	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 (54) 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)
1:A:279:TYR:OH	1:A:295:ARG:NH1	1.99	0.95
1:A:129:ARG:NH1	7:A:601:HOH:O	2.04	0.90
1:A:202:THR:HG22	1:A:204:VAL:H	1.42	0.84
1:A:111:ASN:OD1	1:A:113:GLN:HB2	1.79	0.82
1:A:198:SER:O	1:A:202:THR:HB	1.79	0.81
2:C:3:VAL:N	2:C:26:SER:HG	1.78	0.81
1:B:260[A]:GLN:CD	1:B:260[A]:GLN:H	1.94	0.69
1:B:258:SER:HB2	1:B:260[A]:GLN:OE1	1.94	0.67
1:B:34:GLU:HG3	1:B:35:ASN:HB3	1.77	0.67
1:B:129:ARG:NH1	7:B:601:HOH:O	2.30	0.65
2:C:72:ARG:HD3	2:C:74:ASN:OD1	1.96	0.65
1:B:258:SER:CB	1:B:260[A]:GLN:OE1	2.45	0.64
1:B:398:LYS:HZ1	1:B:409:SER:HG	1.49	0.60
1:B:34:GLU:CG	1:B:35:ASN:HB3	2.35	0.57
2:C:73:ASP:OD2	2:C:76:LYS:HD3	2.04	0.56
1:B:398:LYS:NZ	1:B:409:SER:OG	2.36	0.55
1:B:282:VAL:HG11	1:B:291:MET:HG2	1.88	0.54
1:B:111:ASN:HB3	1:B:113:GLN:HG2	1.88	0.54
1:B:34:GLU:HG2	1:B:35:ASN:N	2.22	0.54
1:B:218:ILE:HD11	1:B:256:PRO:HG2	1.90	0.54
1:A:282:VAL:HG11	1:A:291:MET:HG2	1.90	0.53
1:B:398:LYS:HA	1:B:398:LYS:CE	2.39	0.53
1:A:42:ARG:HG3	1:A:43:TYR:CE2	2.43	0.53
2:C:72:ARG:CD	2:C:74:ASN:OD1	2.56	0.52
1:B:34:GLU:HG3	1:B:35:ASN:CB	2.41	0.51
1:B:34:GLU:CG	1:B:35:ASN:N	2.74	0.51
1:A:240:THR:HG22	1:A:241:THR:N	2.27	0.49
1:A:239:ASN:OD1	1:A:241:THR:HG22	2.11	0.49
1:A:202:THR:HG23	1:A:204:VAL:HG23	1.95	0.49
1:B:273:ILE:HG23	1:B:298:LEU:HD23	1.95	0.48
1:B:218:ILE:HD12	1:B:219:ASP:HB2	1.95	0.48
1:A:156:LEU:C	1:A:156:LEU:HD23	2.34	0.48
1:B:258:SER:OG	1:B:260[A]:GLN:OE1	2.23	0.48
1:B:240:THR:HG22	1:B:241:THR:N	2.29	0.47
1:B:156:LEU:HD23	1:B:156:LEU:C	2.35	0.47
1:A:273:ILE:HG23	1:A:298:LEU:HD23	1.96	0.47
1:A:42:ARG:HG3	1:A:43:TYR:CD2	2.50	0.47
1:A:410:PRO:O	1:A:413:THR:HG23	2.16	0.46
1:A:111:ASN:CG	1:A:113:GLN:HG2	2.37	0.44
2:C:40:GLN:NE2	7:C:201:HOH:O	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:38:TYR:OH	2:C:99:LEU:HD22	2.18	0.43
1:B:410:PRO:O	1:B:413:THR:HG23	2.18	0.42
2:C:83:MET:HB3	2:C:86:LEU:HD21	2.00	0.42
1:A:235:GLN:HA	1:A:235:GLN:OE1	2.19	0.42
1:A:279:TYR:HH	1:A:295:ARG:HH11	1.63	0.42
1:B:218:ILE:O	1:B:219:ASP:C	2.58	0.42
1:B:240:THR:O	1:B:242:ARG:N	2.52	0.42
1:A:111:ASN:N	1:A:111:ASN:OD1	2.45	0.42
1:B:216:GLN:NE2	1:B:218:ILE:HG22	2.35	0.41
1:B:398:LYS:HD3	1:B:398:LYS:HA	1.82	0.41
1:A:82:ALA:HB1	1:A:318:LEU:HD21	2.03	0.41
2:D:83:MET:HB3	2:D:86:LEU:HD21	2.01	0.41
1:B:287:GLY:O	1:B:288:GLY:O	2.39	0.40
2:D:38:TYR:OH	2:D:99:LEU:HD22	2.21	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	411/466 (88%)	396 (96%)	13 (3%)	2 (0%)	34	39
1	B	417/466 (90%)	399 (96%)	13 (3%)	5 (1%)	16	15
2	C	111/120 (92%)	110 (99%)	1 (1%)	0	100	100
2	D	113/120 (94%)	112 (99%)	1 (1%)	0	100	100
All	All	1052/1172 (90%)	1017 (97%)	28 (3%)	7 (1%)	26	30

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	288	GLY

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Mol	Chain	Res	Type
1	B	218	ILE
1	B	219	ASP
1	B	288	GLY
1	B	241	THR
1	A	242	ARG
1	B	289	PRO

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	343/381 (90%)	334 (97%)	9 (3%)	54	69
1	B	347/381 (91%)	336 (97%)	11 (3%)	46	61
2	C	92/99 (93%)	88 (96%)	4 (4%)	35	46
2	D	94/99 (95%)	90 (96%)	4 (4%)	35	46
All	All	876/960 (91%)	848 (97%)	28 (3%)	46	61

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	SER
1	A	145	TYR
1	A	200	LYS
1	A	202	THR
1	A	206	ASP
1	A	227	ILE
1	A	243	VAL
1	A	294	THR
1	A	383	THR
1	B	44	SER
1	B	145	TYR
1	B	178	ASN
1	B	199	LYS
1	B	200	LYS
1	B	206	ASP

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Mol	Chain	Res	Type
1	B	218	ILE
1	B	230	LYS
1	B	243	VAL
1	B	398	LYS
1	B	455	ASP
2	C	14	GLN
2	C	29	ILE
2	C	96	CYS
2	C	99	LEU
2	D	29	ILE
2	D	40	GLN
2	D	96	CYS
2	D	99	LEU

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

Mol	Chain	Res	Type
1	B	216	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](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

10 ligands 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$
3	NAG	A	501	4,6	15,15,15	0.72	0	17,21,21	1.33	2 (11%)
4	GAL	A	502	3,5,6	11,11,12	0.99	1 (9%)	15,15,17	1.43	2 (13%)
5	A2G	A	503	4	14,14,15	0.72	0	15,19,21	1.54	2 (13%)
6	FUC	A	504	4	10,10,11	0.82	0	13,14,16	1.68	4 (30%)
6	FUC	A	505	3	10,10,11	0.77	0	13,14,16	1.75	4 (30%)
3	NAG	B	501	4,6	15,15,15	0.65	0	17,21,21	1.01	1 (5%)
4	GAL	B	502	3,5,6	11,11,12	1.42	2 (18%)	15,15,17	2.80	7 (46%)
5	A2G	B	503	4	14,14,15	0.62	0	15,19,21	1.90	4 (26%)
6	FUC	B	504	4	10,10,11	0.84	0	13,14,16	1.00	1 (7%)
6	FUC	B	505	3	10,10,11	0.71	0	13,14,16	1.40	2 (15%)

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
3	NAG	A	501	4,6	-	0/6/26/26	0/1/1/1
4	GAL	A	502	3,5,6	-	0/2/19/22	0/1/1/1
5	A2G	A	503	4	-	0/6/23/26	0/1/1/1
6	FUC	A	504	4	-	0/0/17/20	0/1/1/1
6	FUC	A	505	3	-	0/0/17/20	0/1/1/1
3	NAG	B	501	4,6	-	0/6/26/26	0/1/1/1
4	GAL	B	502	3,5,6	-	0/2/19/22	0/1/1/1
5	A2G	B	503	4	-	0/6/23/26	0/1/1/1
6	FUC	B	504	4	-	0/0/17/20	0/1/1/1
6	FUC	B	505	3	-	0/0/17/20	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	502	GAL	O5-C1	-2.60	1.39	1.43
4	A	502	GAL	C2-C3	2.22	1.55	1.52
4	B	502	GAL	C2-C3	2.53	1.55	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	502	GAL	O5-C5-C6	-3.47	99.92	107.34
6	A	505	FUC	C2-C3-C4	-2.71	106.32	111.05
6	A	504	FUC	O4-C4-C3	-2.62	104.44	110.36
5	B	503	A2G	C4-C3-C2	-2.50	107.45	111.34
5	A	503	A2G	O6-C6-C5	-2.43	103.20	111.30
4	B	502	GAL	O4-C4-C3	-2.33	105.09	110.36
6	A	505	FUC	C1-C2-C3	-2.15	106.95	109.55
6	A	504	FUC	O5-C1-C2	-2.07	107.58	110.89
3	A	501	NAG	C6-C5-C4	2.01	118.03	112.99
4	B	502	GAL	O5-C1-C2	2.11	114.28	110.89
6	B	504	FUC	C1-C2-C3	2.33	112.38	109.55
6	A	504	FUC	O4-C4-C5	2.40	115.15	109.67
6	B	505	FUC	C1-C2-C3	2.48	112.56	109.55
4	A	502	GAL	O5-C5-C6	2.50	112.69	107.34
3	B	501	NAG	O7-C7-N2	2.51	126.96	121.84
6	A	504	FUC	C1-C2-C3	2.52	112.61	109.55
5	B	503	A2G	C1-O-C5	2.55	115.88	112.14
6	A	505	FUC	O3-C3-C4	2.62	116.27	110.36
6	B	505	FUC	O5-C5-C6	2.70	111.12	106.28
3	A	501	NAG	C3-C4-C5	2.71	115.05	110.23
6	A	505	FUC	O5-C5-C6	3.07	111.78	106.28
4	A	502	GAL	C1-C2-C3	3.10	113.31	109.55
4	B	502	GAL	C3-C4-C5	3.39	116.28	110.23
5	B	503	A2G	O3-C3-C2	3.57	117.01	109.37
5	B	503	A2G	O-C5-C4	3.59	116.08	110.13
5	A	503	A2G	O-C5-C4	3.77	116.37	110.13
4	B	502	GAL	O5-C5-C4	4.21	117.11	110.13
4	B	502	GAL	C1-O5-C5	5.04	119.55	112.14
4	B	502	GAL	C1-C2-C3	5.71	116.47	109.55

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 ⓘ

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, 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	417/466 (89%)	0.08	23 (5%)	29 36	36, 53, 98, 126	0
1	B	420/466 (90%)	0.09	22 (5%)	31 38	37, 56, 103, 121	0
2	C	113/120 (94%)	-0.23	2 (1%)	71 77	39, 53, 72, 102	0
2	D	115/120 (95%)	-0.20	2 (1%)	73 79	33, 45, 66, 105	0
All	All	1065/1172 (90%)	0.02	49 (4%)	36 44	33, 53, 99, 126	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	3	VAL	7.1
1	A	41	THR	6.7
1	A	337	ASN	5.6
1	A	286	SER	5.1
1	A	336	GLY	4.6
1	A	288	GLY	4.6
1	A	338	ASN	4.6
1	B	408	GLY	4.6
1	B	219	ASP	4.4
1	A	408	GLY	4.4
1	A	340	LYS	4.0
1	A	287	GLY	3.7
1	B	238	GLY	3.6
1	B	41	THR	3.4
1	B	338	ASN	3.3
1	A	242	ARG	3.2
1	A	237	LYS	3.2
1	B	42	ARG	3.1
1	B	97	TRP	3.0
1	B	286	SER	3.0
1	B	242	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	238	GLY	2.9
1	A	240	THR	2.9
1	A	289	PRO	2.9
1	A	42	ARG	2.9
1	A	339	GLY	2.8
1	B	94	VAL	2.6
1	B	237	LYS	2.5
1	A	283	THR	2.4
1	B	287	GLY	2.4
1	B	398	LYS	2.4
1	B	329	GLU	2.4
1	B	409	SER	2.4
1	A	409	SER	2.3
1	A	37	SER	2.3
1	A	94	VAL	2.2
2	C	103	ARG	2.2
1	B	269	LEU	2.2
1	B	205	SER	2.2
2	D	99	LEU	2.2
1	B	340	LYS	2.2
1	B	232	VAL	2.1
1	B	288	GLY	2.1
1	B	285	LYS	2.1
1	A	206	ASP	2.1
1	A	217	THR	2.1
1	A	97	TRP	2.1
1	B	220	GLY	2.1
2	D	117	HIS	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](#)

There are no carbohydrates in this entry.

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, 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
3	NAG	A	501	15/15	0.96	0.33	2.80	43,49,53,58	0
5	A2G	A	503	14/15	0.94	0.26	2.53	37,46,52,54	0
5	A2G	B	503	14/15	0.87	0.36	2.36	44,50,69,72	0
6	FUC	B	504	10/11	0.92	0.28	2.15	39,42,44,44	0
6	FUC	A	504	10/11	0.95	0.18	1.33	30,35,37,39	0
3	NAG	B	501	15/15	0.90	0.35	-	44,50,53,54	0
6	FUC	B	505	10/11	0.91	0.47	-	43,44,46,46	0
4	GAL	A	502	11/12	0.91	0.30	-	33,42,47,51	0
4	GAL	B	502	11/12	0.77	0.36	-	38,41,44,48	0
6	FUC	A	505	10/11	0.94	0.42	-	43,49,51,51	0

6.5 Other polymers

There are no such residues in this entry.