



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 04:28 am GMT

PDB ID : 3ZTJ
Title : Structure of influenza A neutralizing antibody selected from cultures of single human plasma cells in complex with human H3 Influenza haemagglutinin.
Authors : Voss, J.E.; Vachieri, S.G.; Gamblin, S.J.; Collins, P.J.; Haire, L.F.; Skehel, J.J.
Deposited on : 2011-07-08
Resolution : 3.41 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

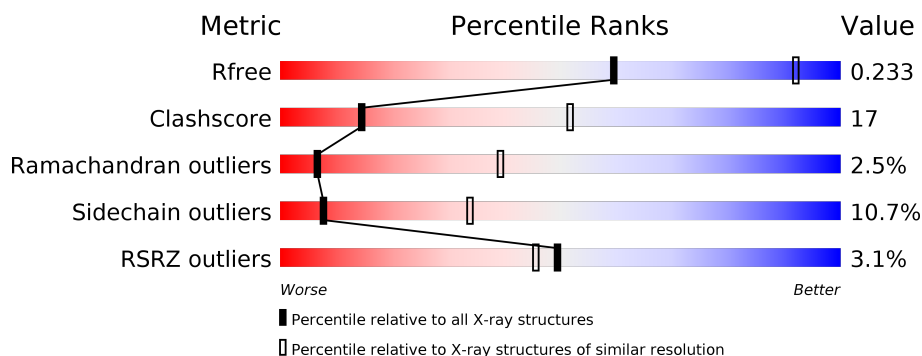
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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}	100719	1074 (3.50-3.34)
Clashscore	112137	1179 (3.50-3.34)
Ramachandran outliers	110173	1147 (3.50-3.34)
Sidechain outliers	110143	1148 (3.50-3.34)
RSRZ outliers	101464	1100 (3.50-3.34)

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	329	<div> <div style="width: 58%; background-color: green;"></div> <div style="width: 34%; background-color: yellow;"></div> <div style="width: 5%; background-color: orange;"></div> <div style="width: 3%; background-color: red;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div>58% 34% 5% .</div>
1	C	329	<div> <div style="width: 53%; background-color: green;"></div> <div style="width: 37%; background-color: yellow;"></div> <div style="width: 5%; background-color: orange;"></div> <div style="width: 3%; background-color: red;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div>53% 37% 5% .</div>
1	E	329	<div> <div style="width: 64%; background-color: green;"></div> <div style="width: 29%; background-color: yellow;"></div> <div style="width: 3%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div>64% 29% . .</div>
2	B	175	<div> <div style="width: 65%; background-color: green;"></div> <div style="width: 29%; background-color: yellow;"></div> <div style="width: 3%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> <div style="width: 1%; background-color: grey;"></div> </div> <div>65% 29% . . .</div>
2	D	175	<div> <div style="width: 59%; background-color: green;"></div> <div style="width: 33%; background-color: yellow;"></div> <div style="width: 6%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> <div style="width: 1%; background-color: grey;"></div> </div> <div>59% 33% 6% .</div>
2	F	175	<div> <div style="width: 66%; background-color: green;"></div> <div style="width: 25%; background-color: yellow;"></div> <div style="width: 6%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> <div style="width: 1%; background-color: grey;"></div> </div> <div>66% 25% 6% . .</div>

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Mol	Chain	Length	Quality of chain
3	G	226	
3	I	226	
3	K	226	
4	H	218	
4	J	218	
4	L	218	

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
5	NAG	A	430	X	-	-	-
6	NAG	C	430	X	-	-	-
6	NAG	F	410	X	-	-	-
7	NAG	D	410	-	-	X	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20384 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 HEMAGGLUTININ HA1 CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2451	1535	430	473	13			
1	C	316	Total	C	N	O	S	0	0	0
			2425	1521	422	469	13			
1	E	318	Total	C	N	O	S	0	0	0
			2451	1535	430	473	13			

- Molecule 2 is a protein called HEMAGGLUTININ HA2 CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1392	863	244	279	6			
2	D	172	Total	C	N	O	S	0	0	0
			1382	856	243	277	6			
2	F	172	Total	C	N	O	S	0	0	0
			1379	854	244	275	6			

- Molecule 3 is a protein called FI6V3 ANTIBODY HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	129	Total	C	N	O	S	0	0	0
			1004	642	167	191	4			
3	I	226	Total	C	N	O	S	0	0	0
			1712	1089	285	332	6			
3	K	224	Total	C	N	O	S	0	0	0
			1697	1082	281	328	6			

- Molecule 4 is a protein called FI6V3 ANTIBODY LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	107	Total	C	N	O	S	0	0	0
			771	485	129	154	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	216	Total	C	N	O	S	0	0	0
			1647	1035	278	329	5			
4	L	216	Total	C	N	O	S	0	0	0
			1623	1018	273	327	5			

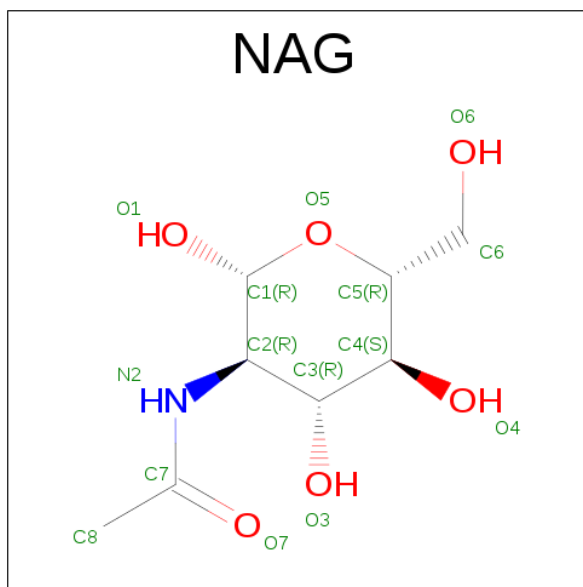
- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			39	22	2	15		
5	A	3	Total	C	N	O	0	0
			39	22	2	15		
5	C	3	Total	C	N	O	0	0
			39	22	2	15		
5	E	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

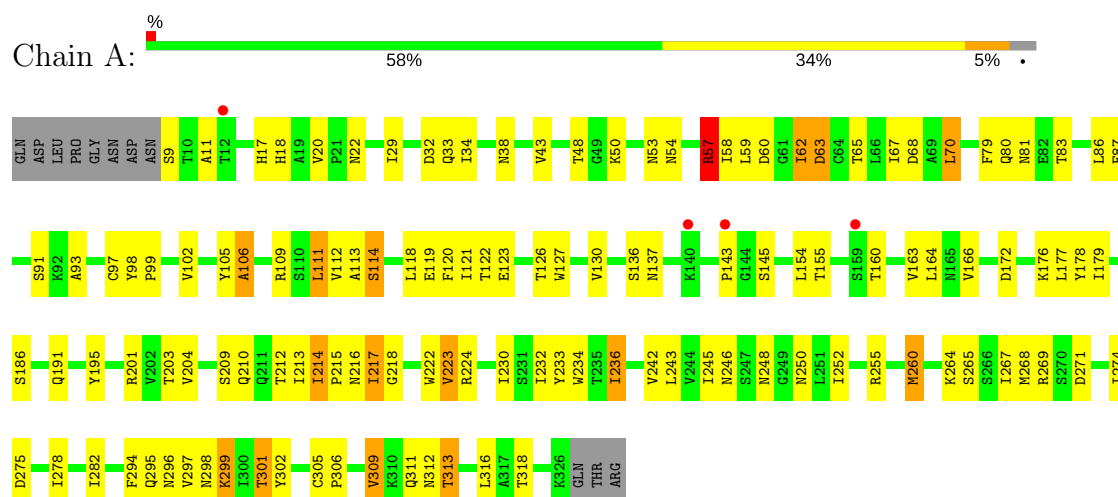


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	N	O	0	0
			14	8	1	5		

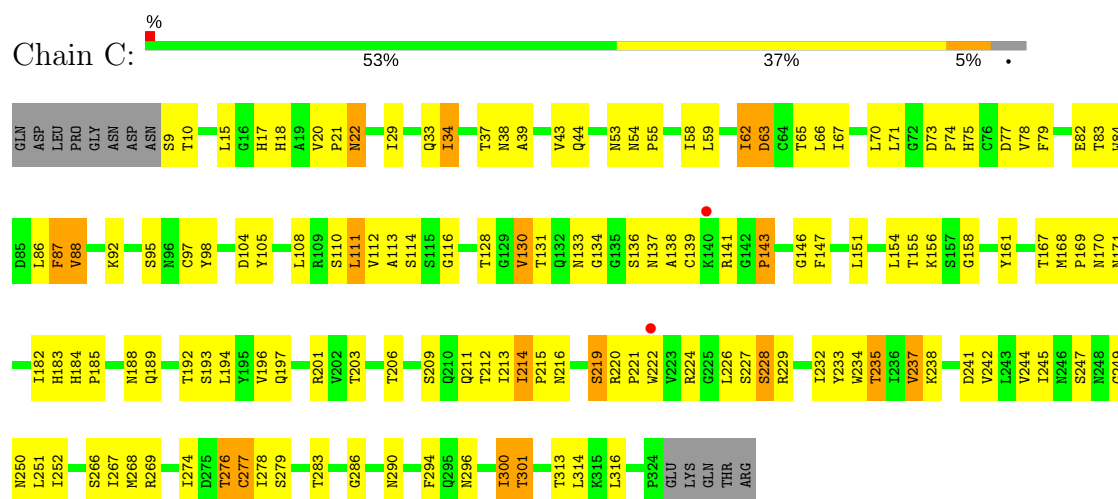
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

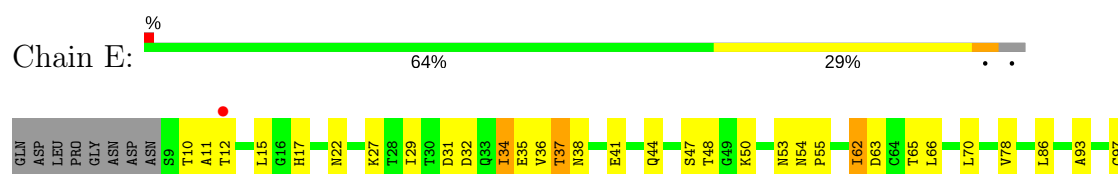
• Molecule 1: HEMAGGLUTININ HA1 CHAIN

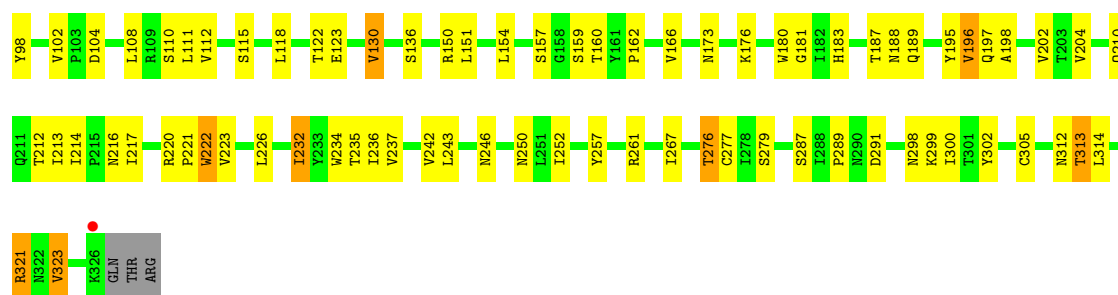


• Molecule 1: HEMAGGLUTININ HA1 CHAIN



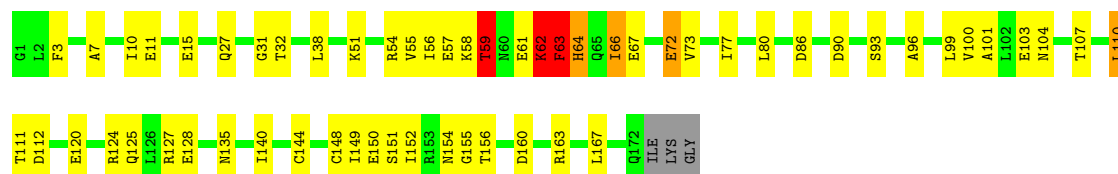
• Molecule 1: HEMAGGLUTININ HA1 CHAIN





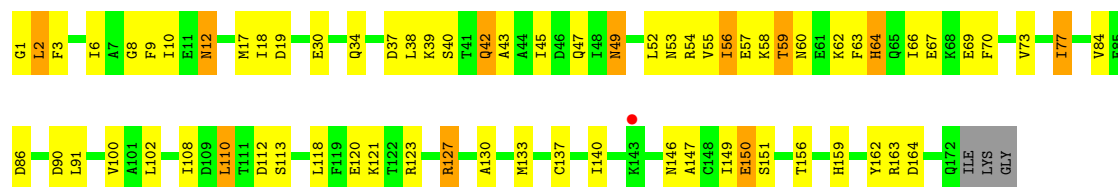
• Molecule 2: HEMAGGLUTININ HA2 CHAIN

Chain B: 65% 29% 6%



• Molecule 2: HEMAGGLUTININ HA2 CHAIN

Chain D: 59% 33% 6%



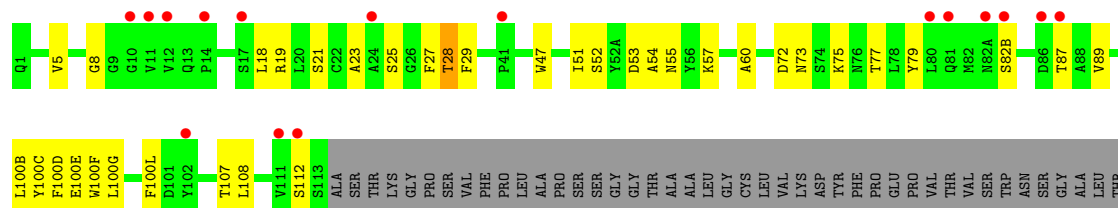
• Molecule 2: HEMAGGLUTININ HA2 CHAIN

Chain F: 66% 25% 6%



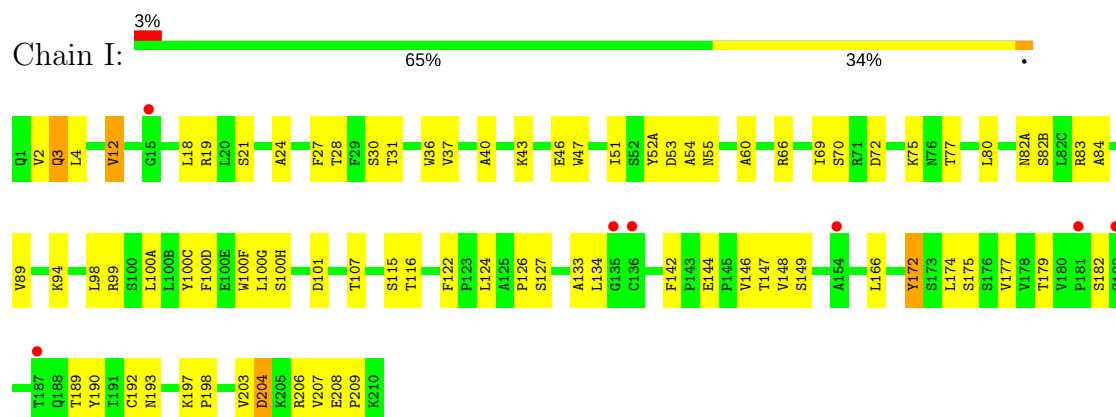
• Molecule 3: FI6V3 ANTIBODY HEAVY CHAIN

Chain G: 41% 15% 43%

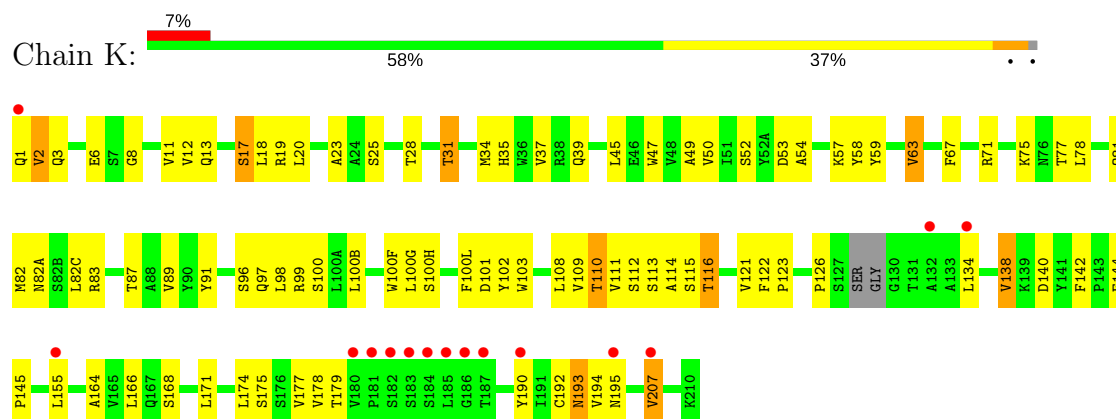


SER GLY VAL HIS THR PHE PRO ALA VAL LEU GLN SER SER GLY TYR SER LEU SER SER VAL VAL THR THR PRO SER SER SER LEU GLY THR GLN THR TYR ILE CYS ASN VAL ASN HIS LYS PRO SER ASN THR LYS VAL ASP LYS ARG VAL GLU PRO LYS

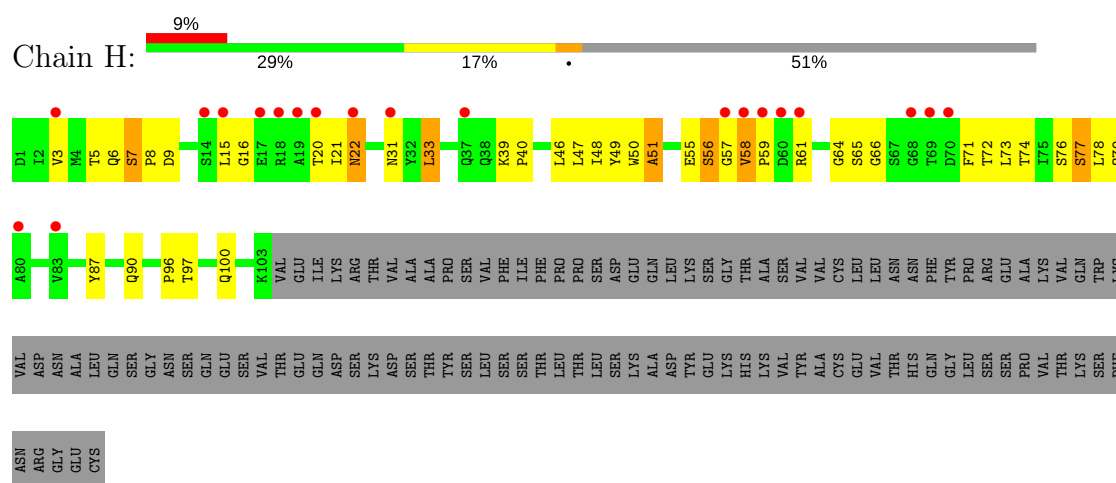
• Molecule 3: FI6V3 ANTIBODY HEAVY CHAIN



• Molecule 3: FI6V3 ANTIBODY HEAVY CHAIN

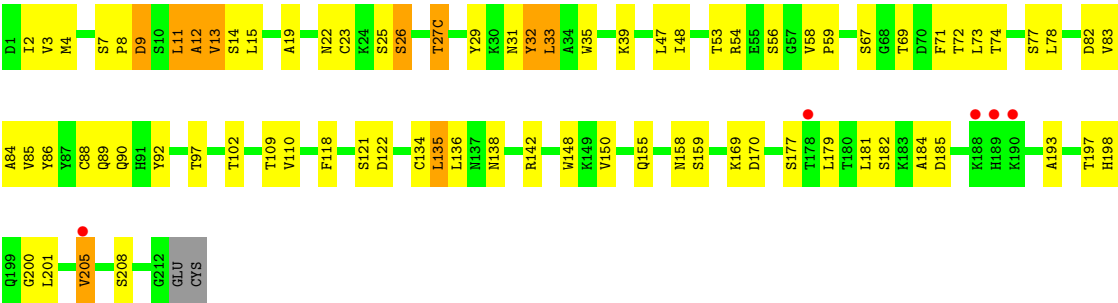


• Molecule 4: FI6V3 ANTIBODY LIGHT CHAIN

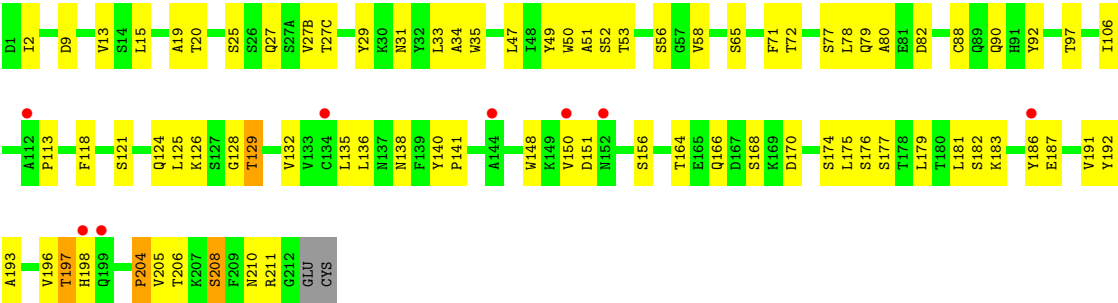


• Molecule 4: FI6V3 ANTIBODY LIGHT CHAIN





● Molecule 4: FI6V3 ANTIBODY LIGHT CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	171.49Å 193.43Å 213.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	143.42 – 3.41 30.16 – 3.41	Depositor EDS
% Data completeness (in resolution range)	95.6 (143.42-3.41) 95.4 (30.16-3.41)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 3.39Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.234 , 0.284 0.236 , 0.233	Depositor DCC
R_{free} test set	4622 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	116.8	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 94.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	20384	wwPDB-VP
Average B, all atoms (Å ²)	152.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% 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: BMA, NAG

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	0.73	0/2507	0.82	1/3417 (0.0%)
1	C	0.78	1/2481 (0.0%)	0.83	0/3384
1	E	0.78	1/2507 (0.0%)	0.86	1/3417 (0.0%)
2	B	0.87	4/1416 (0.3%)	0.82	1/1905 (0.1%)
2	D	0.92	3/1406 (0.2%)	0.87	2/1893 (0.1%)
2	F	0.86	2/1402 (0.1%)	0.85	1/1887 (0.1%)
3	G	0.52	0/1030	0.63	0/1401
3	I	0.67	0/1757	0.73	0/2399
3	K	0.73	0/1741	0.77	0/2376
4	H	0.54	0/792	0.63	0/1088
4	J	0.70	0/1686	0.77	0/2299
4	L	0.61	0/1662	0.71	0/2272
All	All	0.75	11/20387 (0.1%)	0.79	6/27738 (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
2	B	0	1
2	F	0	3
5	A	1	0
6	C	1	0
6	F	1	0
All	All	3	4

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	150	GLU	CB-CG	7.17	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	59	THR	CA-CB	7.02	1.71	1.53
2	D	150	GLU	CG-CD	6.83	1.62	1.51
1	C	277	CYS	CB-SG	6.16	1.92	1.82
2	B	61	GLU	CG-CD	5.71	1.60	1.51

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	63	PHE	N-CA-C	-9.09	86.45	111.00
1	A	57	ARG	NE-CZ-NH1	8.39	124.49	120.30
2	D	54	ARG	NE-CZ-NH1	7.04	123.82	120.30
2	D	54	ARG	NE-CZ-NH2	-6.23	117.19	120.30
2	B	63	PHE	N-CA-CB	5.36	120.25	110.60

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	430	NAG	C1
6	C	430	NAG	C1
6	F	410	NAG	C1

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	62	LYS	Peptide
2	F	57	GLU	Peptide
2	F	62	LYS	Peptide
2	F	75	GLY	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	2451	0	2395	90	0
1	C	2425	0	2364	99	0
1	E	2451	0	2395	68	0
2	B	1392	0	1298	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1382	0	1276	77	0
2	F	1379	0	1285	46	0
3	G	1004	0	937	17	0
3	I	1712	0	1638	68	0
3	K	1697	0	1628	75	0
4	H	771	0	666	30	0
4	J	1647	0	1562	55	0
4	L	1623	0	1497	57	0
5	A	78	0	68	2	0
5	C	39	0	34	0	0
5	E	39	0	34	0	0
6	A	56	0	50	2	0
6	B	28	0	25	1	0
6	C	84	0	75	3	0
6	E	84	0	75	1	0
6	F	28	0	25	2	0
7	D	14	0	13	7	0
All	All	20384	0	19340	682	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 17.

The worst 5 of 682 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:D:52:LEU:O	2:D:56:ILE:HD11	1.43	1.17
2:D:56:ILE:N	2:D:56:ILE:HD12	1.68	1.08
2:D:56:ILE:H	2:D:56:ILE:HD12	1.15	1.00
4:L:13:VAL:HG11	4:L:19:ALA:HB2	1.45	0.98
1:C:53:ASN:HD21	1:C:276:THR:HG23	1.25	0.98

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	316/329 (96%)	276 (87%)	32 (10%)	8 (2%)	6	39
1	C	314/329 (95%)	269 (86%)	36 (12%)	9 (3%)	5	36
1	E	316/329 (96%)	278 (88%)	33 (10%)	5 (2%)	11	49
2	B	170/175 (97%)	143 (84%)	23 (14%)	4 (2%)	7	41
2	D	170/175 (97%)	140 (82%)	23 (14%)	7 (4%)	3	28
2	F	170/175 (97%)	146 (86%)	20 (12%)	4 (2%)	7	41
3	G	127/226 (56%)	109 (86%)	14 (11%)	4 (3%)	5	35
3	I	224/226 (99%)	189 (84%)	33 (15%)	2 (1%)	20	61
3	K	220/226 (97%)	195 (89%)	22 (10%)	3 (1%)	13	51
4	H	105/218 (48%)	81 (77%)	21 (20%)	3 (3%)	5	36
4	J	214/218 (98%)	189 (88%)	19 (9%)	6 (3%)	6	37
4	L	214/218 (98%)	177 (83%)	28 (13%)	9 (4%)	3	27
All	All	2560/2844 (90%)	2192 (86%)	304 (12%)	64 (2%)	6	39

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	ALA
2	D	64	HIS
2	D	127	ARG
2	D	163	ARG
2	F	58	LYS

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	279/290 (96%)	249 (89%)	30 (11%)	7	33
1	C	276/290 (95%)	238 (86%)	38 (14%)	4	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	279/290 (96%)	249 (89%)	30 (11%)	7	33
2	B	145/149 (97%)	134 (92%)	11 (8%)	15	51
2	D	142/149 (95%)	125 (88%)	17 (12%)	6	28
2	F	142/149 (95%)	127 (89%)	15 (11%)	8	34
3	G	102/191 (53%)	95 (93%)	7 (7%)	18	56
3	I	185/191 (97%)	170 (92%)	15 (8%)	14	48
3	K	184/191 (96%)	164 (89%)	20 (11%)	7	33
4	H	74/193 (38%)	65 (88%)	9 (12%)	6	27
4	J	181/193 (94%)	158 (87%)	23 (13%)	5	25
4	L	173/193 (90%)	157 (91%)	16 (9%)	11	41
All	All	2162/2469 (88%)	1931 (89%)	231 (11%)	8	34

5 of 231 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	110	SER
2	F	57	GLU
3	K	193	ASN
1	E	136	SER
1	E	236	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	96	ASN
2	F	53	ASN
4	L	124	GLN
1	E	189	GLN
1	E	216	ASN

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 ⓘ

32 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$
5	NAG	A	430	1,5	14,14,15	0.78	0	15,19,21	1.88	7 (46%)
5	NAG	A	431	5	14,14,15	1.06	1 (7%)	15,19,21	2.00	3 (20%)
5	BMA	A	432	5	11,11,12	1.33	2 (18%)	13,15,17	1.76	4 (30%)
6	NAG	A	440	1,6	14,14,15	1.03	1 (7%)	15,19,21	2.11	6 (40%)
6	NAG	A	441	6	14,14,15	1.27	2 (14%)	15,19,21	2.00	3 (20%)
5	NAG	A	450	1,5	14,14,15	0.74	1 (7%)	15,19,21	1.09	1 (6%)
5	NAG	A	451	5	14,14,15	0.80	0	15,19,21	1.16	3 (20%)
5	BMA	A	452	5	11,11,12	0.94	0	13,15,17	1.92	4 (30%)
6	NAG	A	460	1,6	14,14,15	0.60	0	15,19,21	1.44	4 (26%)
6	NAG	A	461	6	14,14,15	1.30	3 (21%)	15,19,21	1.91	6 (40%)
6	NAG	B	410	2,6	14,14,15	1.24	1 (7%)	15,19,21	1.44	4 (26%)
6	NAG	B	411	6	14,14,15	1.35	2 (14%)	15,19,21	1.88	7 (46%)
6	NAG	C	430	1,6	14,14,15	1.52	2 (14%)	15,19,21	2.95	5 (33%)
6	NAG	C	431	6	14,14,15	1.33	2 (14%)	15,19,21	3.40	7 (46%)
6	NAG	C	440	1,6	14,14,15	1.03	1 (7%)	15,19,21	3.33	8 (53%)
6	NAG	C	441	6	14,14,15	1.37	1 (7%)	15,19,21	2.04	4 (26%)
5	NAG	C	450	1,5	14,14,15	0.61	0	15,19,21	1.86	4 (26%)
5	NAG	C	451	5	14,14,15	0.64	0	15,19,21	1.83	3 (20%)
5	BMA	C	452	5	11,11,12	0.74	0	13,15,17	1.36	2 (15%)
6	NAG	C	460	1,6	14,14,15	0.81	0	15,19,21	1.85	4 (26%)
6	NAG	C	461	6	14,14,15	1.19	1 (7%)	15,19,21	2.39	5 (33%)
6	NAG	E	430	1,6	14,14,15	1.18	2 (14%)	15,19,21	2.63	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	E	431	6	14,14,15	1.30	2 (14%)	15,19,21	2.05	3 (20%)
6	NAG	E	440	1,6	14,14,15	0.88	0	15,19,21	1.83	6 (40%)
6	NAG	E	441	6	14,14,15	1.15	3 (21%)	15,19,21	1.69	3 (20%)
5	NAG	E	450	1,5	14,14,15	0.68	0	15,19,21	1.16	2 (13%)
5	NAG	E	451	5	14,14,15	0.98	1 (7%)	15,19,21	1.07	2 (13%)
5	BMA	E	452	5	11,11,12	1.04	1 (9%)	13,15,17	1.83	6 (46%)
6	NAG	E	460	1,6	14,14,15	1.01	0	15,19,21	2.43	5 (33%)
6	NAG	E	461	6	14,14,15	1.21	1 (7%)	15,19,21	2.00	3 (20%)
6	NAG	F	410	2,6	14,14,15	1.31	1 (7%)	15,19,21	1.57	1 (6%)
6	NAG	F	411	6	14,14,15	0.96	1 (7%)	15,19,21	2.30	4 (26%)

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	430	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	A	431	5	-	0/6/23/26	0/1/1/1
5	BMA	A	432	5	-	0/2/19/22	0/1/1/1
6	NAG	A	440	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	441	6	-	0/6/23/26	0/1/1/1
5	NAG	A	450	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	451	5	-	0/6/23/26	0/1/1/1
5	BMA	A	452	5	-	0/2/19/22	0/1/1/1
6	NAG	A	460	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	461	6	-	0/6/23/26	0/1/1/1
6	NAG	B	410	2,6	-	0/6/23/26	0/1/1/1
6	NAG	B	411	6	-	0/6/23/26	0/1/1/1
6	NAG	C	430	1,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	C	431	6	-	0/6/23/26	0/1/1/1
6	NAG	C	440	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	441	6	-	0/6/23/26	0/1/1/1
5	NAG	C	450	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	451	5	-	0/6/23/26	0/1/1/1
5	BMA	C	452	5	-	0/2/19/22	0/1/1/1
6	NAG	C	460	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	461	6	-	0/6/23/26	0/1/1/1
6	NAG	E	430	1,6	-	0/6/23/26	0/1/1/1
6	NAG	E	431	6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	E	440	1,6	-	0/6/23/26	0/1/1/1
6	NAG	E	441	6	-	0/6/23/26	0/1/1/1
5	NAG	E	450	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	451	5	-	0/6/23/26	0/1/1/1
5	BMA	E	452	5	-	0/2/19/22	0/1/1/1
6	NAG	E	460	1,6	-	0/6/23/26	0/1/1/1
6	NAG	E	461	6	-	0/6/23/26	0/1/1/1
6	NAG	F	410	2,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	F	411	6	-	0/6/23/26	0/1/1/1

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	451	NAG	O5-C1	-2.08	1.40	1.43
5	E	452	BMA	C1-C2	2.00	1.56	1.52
6	A	461	NAG	C2-N2	2.03	1.49	1.46
6	F	411	NAG	C1-C2	2.05	1.55	1.52
6	E	441	NAG	C4-C3	2.15	1.57	1.52

The worst 5 of 134 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	430	NAG	O5-C1-C2	-8.03	100.30	111.47
6	C	440	NAG	O3-C3-C2	-6.91	94.58	109.39
5	C	450	NAG	O5-C1-C2	-4.03	105.86	111.47
6	A	440	NAG	O3-C3-C2	-3.14	102.66	109.39
5	E	450	NAG	C4-C3-C2	-3.06	106.53	111.02

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	430	NAG	C1
6	F	410	NAG	C1
5	A	430	NAG	C1

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	430	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	431	NAG	2	0
6	A	440	NAG	2	0
6	A	441	NAG	2	0
6	B	410	NAG	1	0
6	C	430	NAG	2	0
6	C	431	NAG	2	0
6	C	440	NAG	1	0
6	C	441	NAG	1	0
6	E	440	NAG	1	0
6	E	441	NAG	1	0
6	F	410	NAG	2	0

5.6 Ligand geometry

1 ligand is 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	$\# Z > 2$
7	NAG	D	410	2	14,14,15	1.30	1 (7%)	15,19,21	1.69	3 (20%)

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	NAG	D	410	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	410	NAG	C4-C5	2.78	1.59	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	410	NAG	O5-C1-C2	-3.70	106.32	111.47
7	D	410	NAG	O7-C7-C8	-2.31	117.86	122.06
7	D	410	NAG	C3-C4-C5	3.62	116.60	110.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	410	NAG	7	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	318/329 (96%)	-0.05	4 (1%) 77 73	110, 138, 165, 184	0
1	C	316/329 (96%)	-0.22	2 (0%) 89 86	104, 126, 153, 180	0
1	E	318/329 (96%)	-0.17	2 (0%) 89 86	106, 125, 149, 185	0
2	B	172/175 (98%)	-0.10	0 100 100	98, 143, 196, 219	0
2	D	172/175 (98%)	-0.27	1 (0%) 89 86	97, 135, 196, 233	0
2	F	172/175 (98%)	-0.16	0 100 100	102, 138, 195, 226	0
3	G	129/226 (57%)	0.62	16 (12%) 4 6	163, 221, 268, 289	0
3	I	226/226 (100%)	0.08	7 (3%) 49 45	114, 150, 223, 253	0
3	K	224/226 (99%)	0.10	15 (6%) 19 19	109, 141, 229, 251	0
4	H	107/218 (49%)	0.95	20 (18%) 1 2	189, 240, 266, 273	0
4	J	216/218 (99%)	-0.02	5 (2%) 61 56	113, 142, 196, 223	0
4	L	216/218 (99%)	0.19	8 (3%) 42 38	121, 183, 215, 234	0
All	All	2586/2844 (90%)	0.01	80 (3%) 49 45	97, 140, 233, 289	0

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	10	GLY	6.3
4	H	15	LEU	5.4
3	K	190	TYR	4.3
4	H	14	SER	4.0
4	H	69	THR	3.9

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 ⓘ

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
6	NAG	E	460	14/15	0.92	0.30	1.01	156,164,172,180	0
6	NAG	A	460	14/15	0.92	0.27	0.96	152,160,164,170	0
6	NAG	C	430	14/15	0.86	0.18	0.22	170,180,186,193	0
5	NAG	C	451	14/15	0.93	0.31	0.12	210,221,233,237	0
5	NAG	A	450	14/15	0.96	0.23	-0.05	192,203,213,213	0
6	NAG	E	440	14/15	0.91	0.19	-0.13	162,171,175,184	0
6	NAG	E	430	14/15	0.88	0.18	-0.31	175,187,190,191	0
6	NAG	C	440	14/15	0.83	0.18	-0.31	172,183,192,204	0
5	NAG	A	451	14/15	0.91	0.25	-0.48	209,217,228,228	0
5	NAG	A	430	14/15	0.87	0.17	-0.53	178,188,193,196	0
5	NAG	E	450	14/15	0.96	0.19	-0.57	155,164,168,171	0
5	NAG	C	450	14/15	0.95	0.12	-1.13	183,195,200,203	0
6	NAG	A	440	14/15	0.86	0.15	-1.30	180,186,194,202	0
6	NAG	C	441	14/15	0.84	0.33	-	207,214,219,222	0
6	NAG	E	441	14/15	0.88	0.20	-	191,197,204,209	0
5	BMA	E	452	11/12	0.82	0.19	-	201,205,212,213	0
6	NAG	B	411	14/15	0.76	0.54	-	267,273,284,291	0
5	BMA	A	432	11/12	0.88	0.30	-	214,220,223,226	0
5	BMA	A	452	11/12	0.60	0.20	-	230,232,237,240	0
6	NAG	E	431	14/15	0.89	0.23	-	190,200,204,205	0
6	NAG	C	461	14/15	0.93	0.33	-	167,171,175,178	0
6	NAG	C	460	14/15	0.95	0.24	-	143,149,159,160	0
6	NAG	C	431	14/15	0.70	0.34	-	200,206,210,215	0
6	NAG	F	411	14/15	0.81	0.49	-	258,264,271,277	0
6	NAG	A	441	14/15	0.91	0.17	-	212,217,225,226	0
5	NAG	E	451	14/15	0.92	0.23	-	177,183,195,196	0
6	NAG	A	461	14/15	0.82	0.34	-	181,188,190,191	0
6	NAG	E	461	14/15	0.88	0.40	-	190,196,203,203	0
6	NAG	F	410	14/15	0.85	0.30	-	223,239,248,250	0
5	BMA	C	452	11/12	0.61	0.21	-	243,248,254,258	0
5	NAG	A	431	14/15	0.88	0.23	-	197,203,217,217	0
6	NAG	B	410	14/15	0.71	0.29	-	232,248,258,261	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, 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
7	NAG	D	410	14/15	0.61	0.37	2.11	201,215,222,225	0

6.5 Other polymers [i](#)

There are no such residues in this entry.