



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 10:31 PM BST

PDB ID : 6OEJ
Title : CRYSTAL STRUCTURE OF THE NON-NEUTRALIZING AND ADCC-POTENT ANTIBODY C11 IN COMPLEX WITH HIV-1 CLADE A/E GP120
Authors : Tolbert, W.D.; Pazgier, M.
Deposited on : 2019-03-27
Resolution : 3.45 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

<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

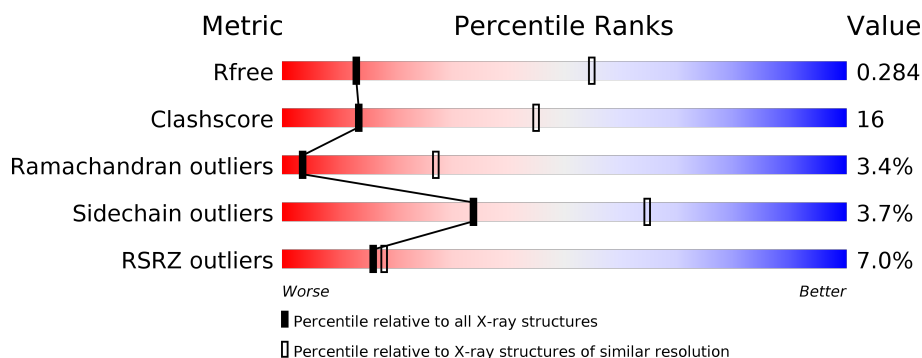
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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 $\leq 5\%$. 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	385	<div> <div>13%</div> <div>51%</div> <div>30%</div> <div>•</div> <div>16%</div> </div>
1	G	385	<div> <div>10%</div> <div>49%</div> <div>31%</div> <div>•</div> <div>17%</div> </div>
2	B	239	<div> <div>3%</div> <div>59%</div> <div>35%</div> <div>•</div> <div>5%</div> </div>
2	H	239	<div> <div>3%</div> <div>61%</div> <div>31%</div> <div>•</div> <div>5%</div> </div>
3	C	218	<div> <div>%</div> <div>59%</div> <div>34%</div> <div>•</div> <div>6%</div> </div>
3	L	218	<div> <div>%</div> <div>75%</div> <div>22%</div> <div>••</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	4	
4	E	4	

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	610	-	-	-	X
5	NAG	G	608	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12140 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 clade A/E 93TH057 HIV-1 gp120 core.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	319	Total	C	N	O	S	0	0	0
			2497	1574	423	478	22			
1	A	322	Total	C	N	O	S	0	0	0
			2524	1591	429	481	23			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	31	CYS	-	see sequence details	UNP A0A0M3KKW9
G	32	ASP	-	see sequence details	UNP A0A0M3KKW9
G	33	ASN	-	see sequence details	UNP A0A0M3KKW9
G	34	LEU	-	see sequence details	UNP A0A0M3KKW9
G	35	TRP	-	see sequence details	UNP A0A0M3KKW9
G	36	VAL	-	see sequence details	UNP A0A0M3KKW9
G	37	THR	-	see sequence details	UNP A0A0M3KKW9
G	38	VAL	-	see sequence details	UNP A0A0M3KKW9
G	39	TYR	-	see sequence details	UNP A0A0M3KKW9
G	40	TYR	-	see sequence details	UNP A0A0M3KKW9
G	41	GLY	-	see sequence details	UNP A0A0M3KKW9
G	42	VAL	-	see sequence details	UNP A0A0M3KKW9
G	43	PRO	-	see sequence details	UNP A0A0M3KKW9
G	80	CYS	ASN	engineered mutation	UNP A0A0M3KKW9
G	375	SER	HIS	engineered mutation	UNP A0A0M3KKW9
G	493	PRO	-	see sequence details	UNP A0A0M3KKW9
G	494	LEU	-	see sequence details	UNP A0A0M3KKW9
G	495	GLY	-	see sequence details	UNP A0A0M3KKW9
G	496	ILE	-	see sequence details	UNP A0A0M3KKW9
G	497	ALA	-	see sequence details	UNP A0A0M3KKW9
G	498	PRO	-	see sequence details	UNP A0A0M3KKW9
G	499	THR	-	see sequence details	UNP A0A0M3KKW9
G	500	LYS	-	see sequence details	UNP A0A0M3KKW9
G	501	ALA	-	see sequence details	UNP A0A0M3KKW9
G	502	LYS	-	see sequence details	UNP A0A0M3KKW9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	503	ARG	-	see sequence details	UNP A0A0M3KKW9
G	504	ARG	-	see sequence details	UNP A0A0M3KKW9
G	505	VAL	-	see sequence details	UNP A0A0M3KKW9
G	506	VAL	-	see sequence details	UNP A0A0M3KKW9
G	507	GLN	-	see sequence details	UNP A0A0M3KKW9
G	508	ARG	-	see sequence details	UNP A0A0M3KKW9
G	509	GLU	-	see sequence details	UNP A0A0M3KKW9
G	510	LYS	-	see sequence details	UNP A0A0M3KKW9
G	511	ARG	-	see sequence details	UNP A0A0M3KKW9
A	31	CYS	-	see sequence details	UNP A0A0M3KKW9
A	32	ASP	-	see sequence details	UNP A0A0M3KKW9
A	33	ASN	-	see sequence details	UNP A0A0M3KKW9
A	34	LEU	-	see sequence details	UNP A0A0M3KKW9
A	35	TRP	-	see sequence details	UNP A0A0M3KKW9
A	36	VAL	-	see sequence details	UNP A0A0M3KKW9
A	37	THR	-	see sequence details	UNP A0A0M3KKW9
A	38	VAL	-	see sequence details	UNP A0A0M3KKW9
A	39	TYR	-	see sequence details	UNP A0A0M3KKW9
A	40	TYR	-	see sequence details	UNP A0A0M3KKW9
A	41	GLY	-	see sequence details	UNP A0A0M3KKW9
A	42	VAL	-	see sequence details	UNP A0A0M3KKW9
A	43	PRO	-	see sequence details	UNP A0A0M3KKW9
A	80	CYS	ASN	engineered mutation	UNP A0A0M3KKW9
A	375	SER	HIS	engineered mutation	UNP A0A0M3KKW9
A	493	PRO	-	see sequence details	UNP A0A0M3KKW9
A	494	LEU	-	see sequence details	UNP A0A0M3KKW9
A	495	GLY	-	see sequence details	UNP A0A0M3KKW9
A	496	ILE	-	see sequence details	UNP A0A0M3KKW9
A	497	ALA	-	see sequence details	UNP A0A0M3KKW9
A	498	PRO	-	see sequence details	UNP A0A0M3KKW9
A	499	THR	-	see sequence details	UNP A0A0M3KKW9
A	500	LYS	-	see sequence details	UNP A0A0M3KKW9
A	501	ALA	-	see sequence details	UNP A0A0M3KKW9
A	502	LYS	-	see sequence details	UNP A0A0M3KKW9
A	503	ARG	-	see sequence details	UNP A0A0M3KKW9
A	504	ARG	-	see sequence details	UNP A0A0M3KKW9
A	505	VAL	-	see sequence details	UNP A0A0M3KKW9
A	506	VAL	-	see sequence details	UNP A0A0M3KKW9
A	507	GLN	-	see sequence details	UNP A0A0M3KKW9
A	508	ARG	-	see sequence details	UNP A0A0M3KKW9
A	509	GLU	-	see sequence details	UNP A0A0M3KKW9
A	510	LYS	-	see sequence details	UNP A0A0M3KKW9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	511	ARG	-	see sequence details	UNP A0A0M3KKW9

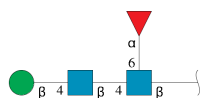
- Molecule 2 is a protein called C11 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	227	Total	C	N	O	S	0	0	0
			1708	1079	288	334	7			
2	B	227	Total	C	N	O	S	0	0	0
			1709	1079	288	335	7			

- Molecule 3 is a protein called C11 Fab light chain.

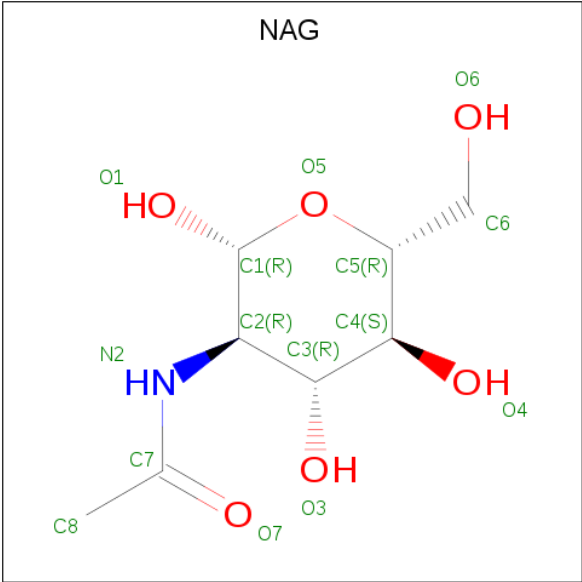
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	215	Total	C	N	O	S	0	0	0
			1646	1035	277	328	6			
3	C	216	Total	C	N	O	S	0	0	0
			1650	1037	278	329	6			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	4	Total	C	N	O	0	0	0
			49	28	2	19			
4	E	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

Continued on next page...

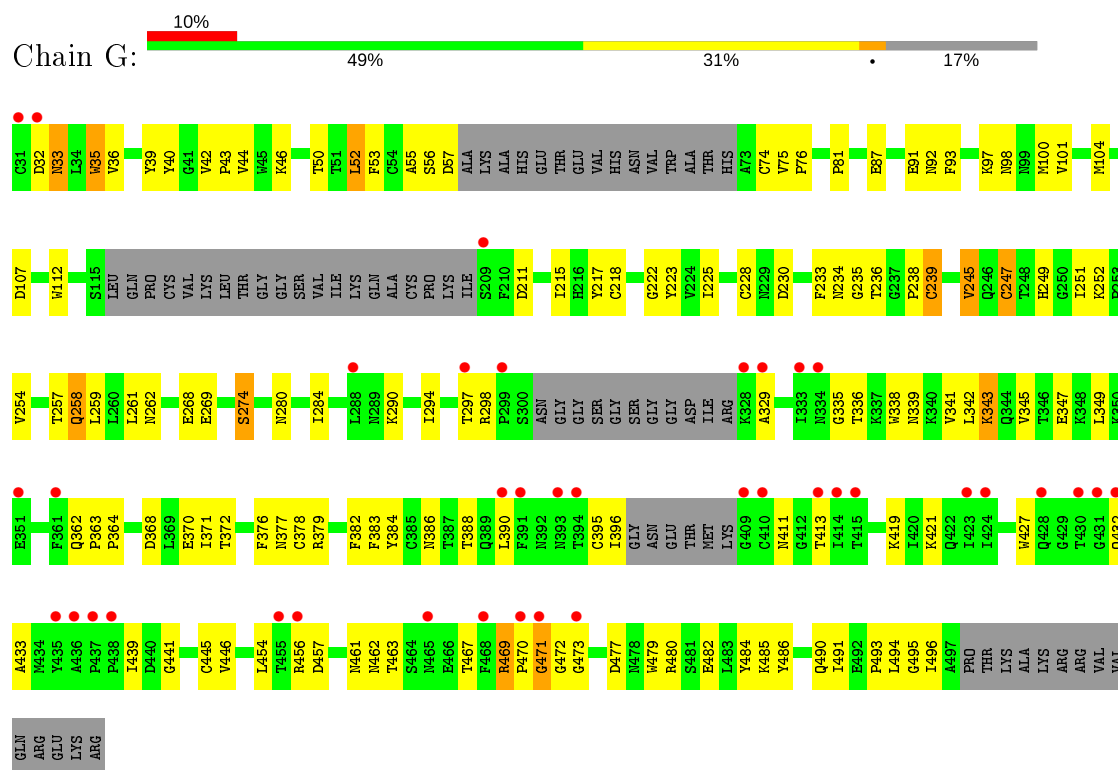
Continued from previous page...

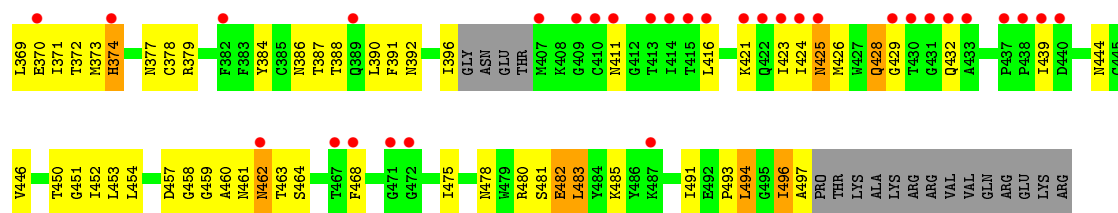
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots

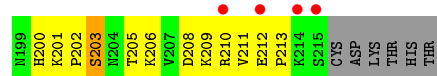
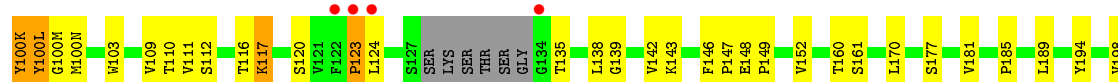
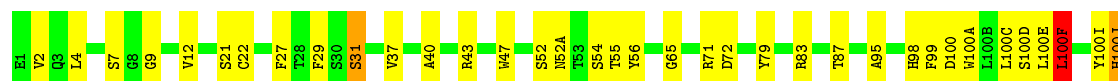
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: clade A/E 93TH057 HIV-1 gp120 core





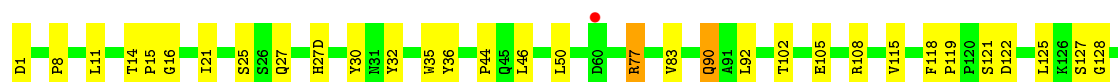
• Molecule 2: C11 Fab heavy chain



• Molecule 2: C11 Fab heavy chain

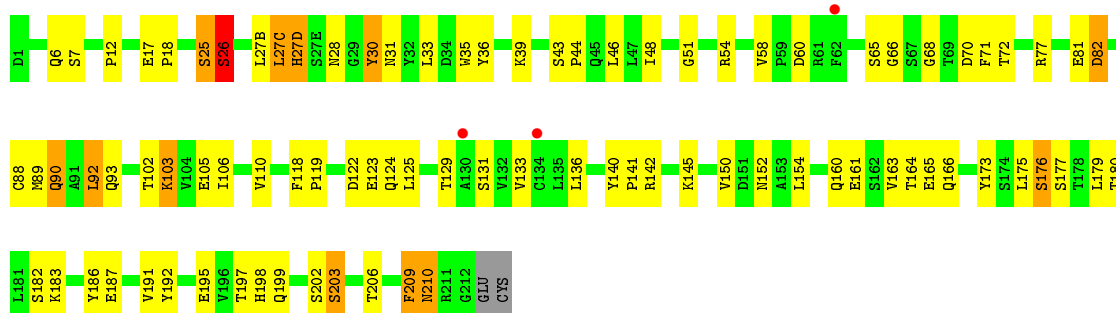


• Molecule 3: C11 Fab light chain



• Molecule 3: C11 Fab light chain





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

Chain D: 50% 50%



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

Chain E: 75% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.37Å 110.96Å 217.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.42 – 3.45 49.42 – 3.45	Depositor EDS
% Data completeness (in resolution range)	91.1 (49.42-3.45) 91.2 (49.42-3.45)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.13 _2998: ???)	Depositor
R, R_{free}	0.231 , 0.284 0.231 , 0.284	Depositor DCC
R_{free} test set	1313 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	98.9	Xtriage
Anisotropy	0.773	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12140	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% 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, FUC

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	0.27	0/2577	0.50	0/3498
1	G	0.28	0/2549	0.52	0/3462
2	B	0.28	0/1751	0.53	0/2385
2	H	0.31	0/1750	0.56	1/2384 (0.0%)
3	C	0.33	0/1686	0.60	3/2290 (0.1%)
3	L	0.28	0/1682	0.52	0/2285
All	All	0.29	0/11995	0.53	4/16304 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	100(F)	LEU	CB-CG-CD1	8.37	125.22	111.00
3	C	27(C)	LEU	CB-CG-CD2	6.91	122.74	111.00
3	C	27(C)	LEU	CB-CG-CD1	6.51	122.06	111.00
3	C	30	TYR	CA-CB-CG	5.91	124.63	113.40

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	2524	0	2446	89	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2497	0	2417	97	1
2	B	1709	0	1649	65	0
2	H	1708	0	1646	65	1
3	C	1650	0	1617	62	0
3	L	1646	0	1614	35	0
4	D	49	0	43	1	0
4	E	49	0	43	0	0
5	A	154	0	143	4	0
5	G	154	0	143	2	0
All	All	12140	0	11761	383	1

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 16.

The worst 5 of 383 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)
3:C:90:GLN:OE1	3:C:92:LEU:N	1.88	1.06
2:H:100:ASP:OD2	3:L:27(D):HIS:NE2	1.91	1.02
3:C:195:GLU:HG2	3:C:206:THR:HB	1.58	0.85
2:H:87:THR:HG23	2:H:110:THR:HA	1.59	0.84
2:B:52(A):ASN:HA	2:B:71:ARG:HH12	1.43	0.83

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:368:ASP:OD1	2:H:160:THR:N[2_455]	2.16	0.04

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	312/385 (81%)	260 (83%)	37 (12%)	15 (5%)	2	19
1	G	309/385 (80%)	256 (83%)	45 (15%)	8 (3%)	5	32
2	B	223/239 (93%)	183 (82%)	34 (15%)	6 (3%)	5	31
2	H	223/239 (93%)	176 (79%)	39 (18%)	8 (4%)	3	25
3	C	214/218 (98%)	175 (82%)	31 (14%)	8 (4%)	3	25
3	L	213/218 (98%)	183 (86%)	24 (11%)	6 (3%)	5	31
All	All	1494/1684 (89%)	1233 (82%)	210 (14%)	51 (3%)	3	27

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	36	VAL
2	H	100(J)	HIS
2	H	100(K)	TYR
2	H	117	LYS
2	H	123	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	289/339 (85%)	283 (98%)	6 (2%)	53	78
1	G	286/339 (84%)	277 (97%)	9 (3%)	40	70
2	B	189/202 (94%)	184 (97%)	5 (3%)	46	74
2	H	188/202 (93%)	179 (95%)	9 (5%)	25	58
3	C	188/190 (99%)	173 (92%)	15 (8%)	12	40
3	L	188/190 (99%)	183 (97%)	5 (3%)	44	73
All	All	1328/1462 (91%)	1279 (96%)	49 (4%)	34	64

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	176	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	478	ASN
3	C	176	SER
1	A	298	ARG
1	A	494	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
3	L	198	HIS
3	C	31	ASN
1	A	374	HIS
2	H	35	ASN
3	C	27(D)	HIS

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 ⓘ

8 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	$\# Z > 2$
4	NAG	D	1	2,4	14,14,15	0.28	0	17,19,21	0.51	0
4	NAG	D	2	4	14,14,15	0.54	0	17,19,21	0.49	0
4	BMA	D	3	4	11,11,12	0.67	0	15,15,17	0.78	0
4	FUC	D	4	4	10,10,11	0.82	0	14,14,16	1.01	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	E	1	2,4	14,14,15	0.26	0	17,19,21	0.54	0
4	NAG	E	2	4	14,14,15	0.20	0	17,19,21	0.53	0
4	BMA	E	3	4	11,11,12	0.59	0	15,15,17	0.79	0
4	FUC	E	4	4	10,10,11	0.83	0	14,14,16	1.33	2 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	4/6/23/26	0/1/1/1
4	BMA	D	3	4	-	2/2/19/22	0/1/1/1
4	FUC	D	4	4	-	-	0/1/1/1
4	NAG	E	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	1/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	FUC	E	4	4	-	-	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	4	FUC	O5-C5-C4	3.04	114.97	109.52
4	E	4	FUC	C1-O5-C5	2.22	117.81	112.78
4	D	4	FUC	O5-C5-C4	2.22	113.50	109.52

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	D	3	BMA	C4-C5-C6-O6
4	D	2	NAG	C1-C2-N2-C7
4	D	3	BMA	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2	NAG	1	0

5.6 Ligand geometry

22 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$
5	NAG	A	602	1	14,14,15	0.47	0	17,19,21	0.42	0
5	NAG	A	604	1	14,14,15	0.44	0	17,19,21	0.51	0
5	NAG	A	609	1	14,14,15	0.29	0	17,19,21	0.58	0
5	NAG	G	611	1	14,14,15	0.29	0	17,19,21	0.47	0
5	NAG	A	611	1	14,14,15	0.22	0	17,19,21	0.37	0
5	NAG	G	603	1	14,14,15	0.27	0	17,19,21	0.36	0
5	NAG	A	610	1	14,14,15	0.35	0	17,19,21	0.45	0
5	NAG	A	603	1	14,14,15	0.39	0	17,19,21	0.54	0
5	NAG	G	608	1	14,14,15	0.23	0	17,19,21	0.47	0
5	NAG	G	606	1	14,14,15	0.30	0	17,19,21	0.46	0
5	NAG	G	609	1	14,14,15	0.37	0	17,19,21	0.49	0
5	NAG	G	605	1	14,14,15	0.35	0	17,19,21	0.33	0
5	NAG	A	606	1	14,14,15	0.34	0	17,19,21	0.34	0
5	NAG	A	607	1	14,14,15	0.20	0	17,19,21	0.47	0
5	NAG	G	604	1	14,14,15	0.27	0	17,19,21	0.40	0
5	NAG	A	608	1	14,14,15	0.30	0	17,19,21	0.40	0
5	NAG	G	601	1	14,14,15	0.41	0	17,19,21	0.52	0
5	NAG	A	601	1	14,14,15	0.72	1 (7%)	17,19,21	0.67	0
5	NAG	A	605	1	14,14,15	0.39	0	17,19,21	0.48	0
5	NAG	G	602	1	14,14,15	0.40	0	17,19,21	0.39	0
5	NAG	G	607	1	14,14,15	0.37	0	17,19,21	0.51	0
5	NAG	G	610	1	14,14,15	0.32	0	17,19,21	0.49	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	602	1	-	1/6/23/26	0/1/1/1
5	NAG	A	604	1	-	2/6/23/26	0/1/1/1
5	NAG	A	609	1	-	2/6/23/26	0/1/1/1
5	NAG	G	611	1	-	2/6/23/26	0/1/1/1
5	NAG	A	611	1	-	2/6/23/26	0/1/1/1
5	NAG	G	603	1	-	2/6/23/26	0/1/1/1
5	NAG	A	610	1	-	0/6/23/26	0/1/1/1
5	NAG	A	603	1	-	0/6/23/26	0/1/1/1
5	NAG	G	608	1	-	2/6/23/26	0/1/1/1
5	NAG	G	606	1	-	2/6/23/26	0/1/1/1
5	NAG	G	609	1	-	1/6/23/26	0/1/1/1
5	NAG	G	605	1	-	3/6/23/26	0/1/1/1
5	NAG	A	606	1	-	2/6/23/26	0/1/1/1
5	NAG	A	607	1	-	2/6/23/26	0/1/1/1
5	NAG	G	604	1	-	2/6/23/26	0/1/1/1
5	NAG	A	608	1	-	1/6/23/26	0/1/1/1
5	NAG	G	601	1	-	1/6/23/26	0/1/1/1
5	NAG	A	601	1	-	2/6/23/26	0/1/1/1
5	NAG	A	605	1	-	1/6/23/26	0/1/1/1
5	NAG	G	602	1	-	0/6/23/26	0/1/1/1
5	NAG	G	607	1	-	0/6/23/26	0/1/1/1
5	NAG	G	610	1	-	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)
5	A	601	NAG	C1-C2	2.56	1.56	1.52

There are no bond angle outliers.

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	608	NAG	C4-C5-C6-O6
5	A	611	NAG	O5-C5-C6-O6
5	G	603	NAG	O5-C5-C6-O6
5	A	607	NAG	O5-C5-C6-O6
5	G	608	NAG	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	604	NAG	1	0
5	A	609	NAG	1	0
5	A	610	NAG	1	0
5	G	604	NAG	1	0
5	A	601	NAG	1	0
5	G	602	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	322/385 (83%)	0.78	50 (15%) 2 3	78, 156, 204, 235	0
1	G	319/385 (82%)	0.62	38 (11%) 4 6	73, 145, 199, 257	0
2	B	227/239 (94%)	0.07	6 (2%) 56 53	51, 84, 124, 147	0
2	H	227/239 (94%)	0.09	8 (3%) 44 42	50, 83, 126, 142	0
3	C	216/218 (99%)	0.08	3 (1%) 75 72	52, 86, 115, 129	0
3	L	215/218 (98%)	0.04	2 (0%) 84 81	52, 86, 118, 135	0
All	All	1526/1684 (90%)	0.34	107 (7%) 16 18	50, 101, 194, 257	0

The worst 5 of 107 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	436	ALA	11.2
1	A	424	ILE	8.5
1	A	31	CYS	7.6
2	H	215	SER	6.7
1	G	471	GLY	6.5

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. 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	B-factors(\AA^2)	Q<0.9
4	BMA	E	3	11/12	0.76	0.20	195,204,214,217	0
4	BMA	D	3	11/12	0.79	0.22	178,196,200,202	0
4	NAG	D	2	14/15	0.88	0.22	145,166,170,177	0
4	NAG	E	2	14/15	0.88	0.20	141,165,174,185	0
4	NAG	E	1	14/15	0.88	0.16	73,102,122,124	0
4	FUC	D	4	10/11	0.92	0.22	71,104,115,121	0
4	NAG	D	1	14/15	0.93	0.16	77,93,117,132	0
4	FUC	E	4	10/11	0.93	0.27	68,108,125,136	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. 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	B-factors(\AA^2)	Q<0.9
5	NAG	G	610	14/15	0.52	0.39	238,259,269,284	0
5	NAG	A	606	14/15	0.62	0.37	132,155,166,175	0
5	NAG	A	610	14/15	0.71	0.49	159,178,197,199	0
5	NAG	A	605	14/15	0.71	0.25	185,191,194,197	0
5	NAG	G	609	14/15	0.71	0.39	182,191,197,197	0
5	NAG	A	609	14/15	0.72	0.34	206,213,219,221	0
5	NAG	A	608	14/15	0.72	0.39	161,206,214,217	0
5	NAG	G	608	14/15	0.73	0.41	167,200,208,209	0
5	NAG	A	601	14/15	0.74	0.29	124,150,165,165	0
5	NAG	G	601	14/15	0.75	0.25	148,178,192,193	0
5	NAG	A	602	14/15	0.77	0.36	135,184,195,201	0
5	NAG	G	602	14/15	0.78	0.31	149,169,186,193	0
5	NAG	G	611	14/15	0.78	0.34	139,158,166,168	0
5	NAG	G	607	14/15	0.81	0.21	160,172,183,183	0
5	NAG	G	606	14/15	0.82	0.21	120,140,144,147	0
5	NAG	A	604	14/15	0.83	0.25	101,117,145,147	0
5	NAG	A	607	14/15	0.84	0.27	149,168,174,175	0
5	NAG	A	611	14/15	0.89	0.36	131,156,171,174	0
5	NAG	A	603	14/15	0.89	0.21	90,107,120,128	0
5	NAG	G	605	14/15	0.90	0.18	137,150,160,162	0
5	NAG	G	603	14/15	0.91	0.22	99,121,142,145	0
5	NAG	G	604	14/15	0.92	0.16	115,133,151,156	0

6.5 Other polymers [i](#)

There are no such residues in this entry.