



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 28, 2022 – 12:08 PM EDT

PDB ID : 7N8Q  
Title : Rhesusized RV305 DH677.3 Fab bound to Clade A/E 93TH057 HIV-1 gp120 core.  
Authors : Tolbert, W.D.; Pazgier, M.  
Deposited on : 2021-06-15  
Resolution : 2.90 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](mailto: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.

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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	:	2.27
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)	:	2.27

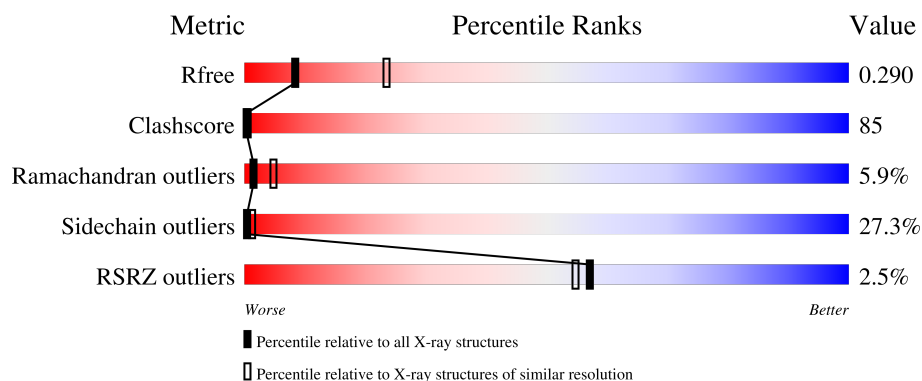
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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.



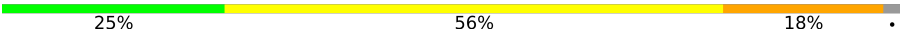
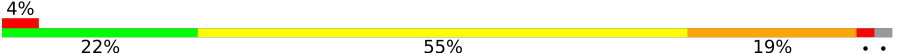
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	355	 3% 22% 43% 21% 13%
1	G	355	 2% 23% 54% 18% 5%
2	N	28	 4% 57% 32% 11%
3	C	228	 3% 28% 50% 17% 5%
3	H	228	 3% 25% 52% 18%

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Mol	Chain	Length	Quality of chain
4	D	214	
4	L	214	

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	G	509	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12057 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	338	Total	C	N	O	S	0	0	0
			2646	1663	458	503	22			
1	A	308	Total	C	N	O	S	0	0	0
			2419	1516	417	465	21			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	42	VAL	-	expression tag	UNP A0A0M3KKW9
G	43	PRO	-	expression tag	UNP A0A0M3KKW9
G	375	SER	HIS	engineered mutation	UNP A0A0M3KKW9
A	42	VAL	-	expression tag	UNP A0A0M3KKW9
A	43	PRO	-	expression tag	UNP A0A0M3KKW9
A	375	SER	HIS	engineered mutation	UNP A0A0M3KKW9

- Molecule 2 is a protein called M48U1 CD4 MIMETIC PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	28	Total	C	N	O	S	0	0	1
			209	133	38	32	6			

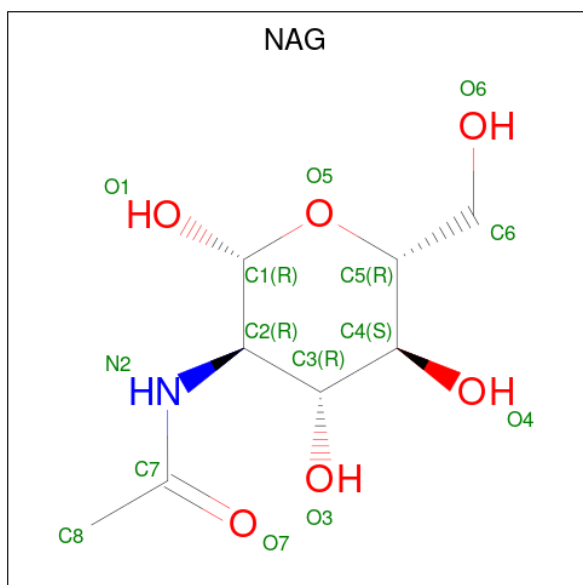
- Molecule 3 is a protein called Rhesusized DH677.3 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	218	Total	C	N	O	S	0	0	0
			1657	1049	277	323	8			
3	C	217	Total	C	N	O	S	0	0	0
			1651	1046	276	321	8			

- Molecule 4 is a protein called Rhesusized DH677.3 FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	210	Total	C	N	O	S	0	0	0
			1604	1008	266	325	5			
4	D	210	Total	C	N	O	S	0	0	0
			1604	1008	266	325	5			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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		

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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		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

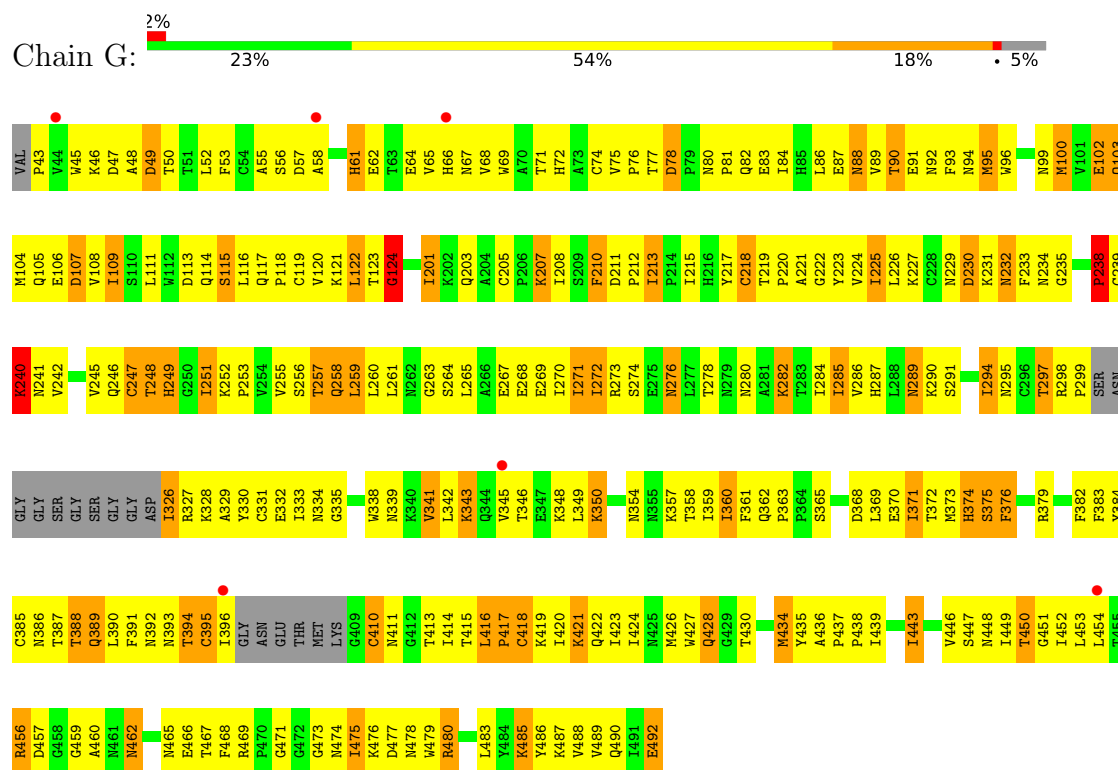
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	5	Total	O	0	0
			5	5		
6	H	3	Total	O	0	0
			3	3		
6	L	2	Total	O	0	0
			2	2		
6	A	2	Total	O	0	0
			2	2		
6	C	1	Total	O	0	0
			1	1		
6	D	2	Total	O	0	0
			2	2		

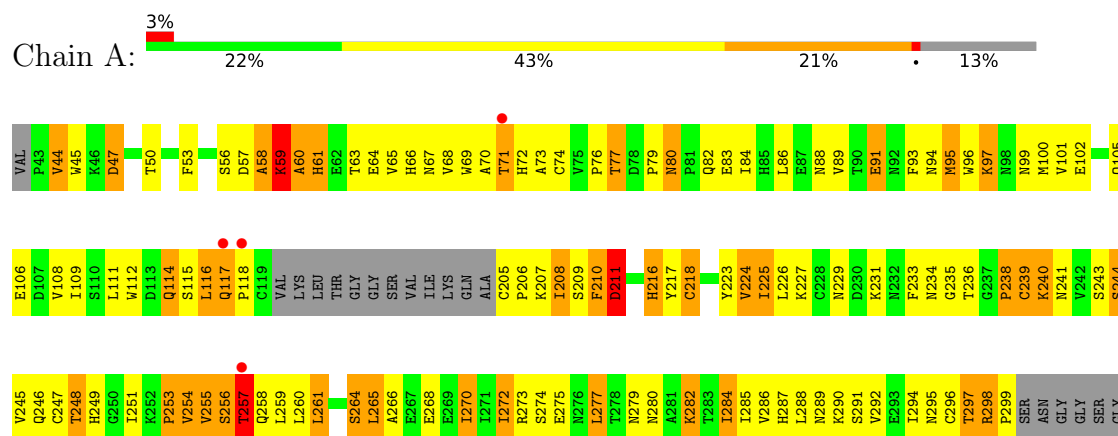
### 3 Residue-property plots

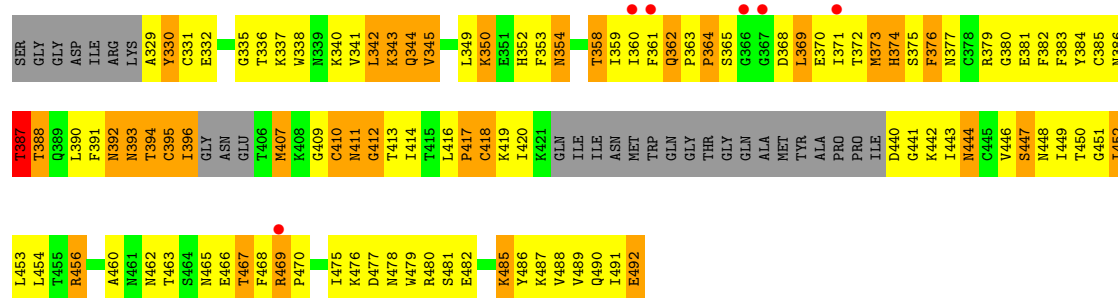
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

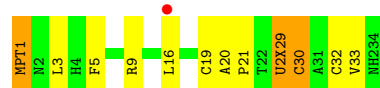


- Molecule 1: clade A/E 93TH057 HIV-1 gp120 core

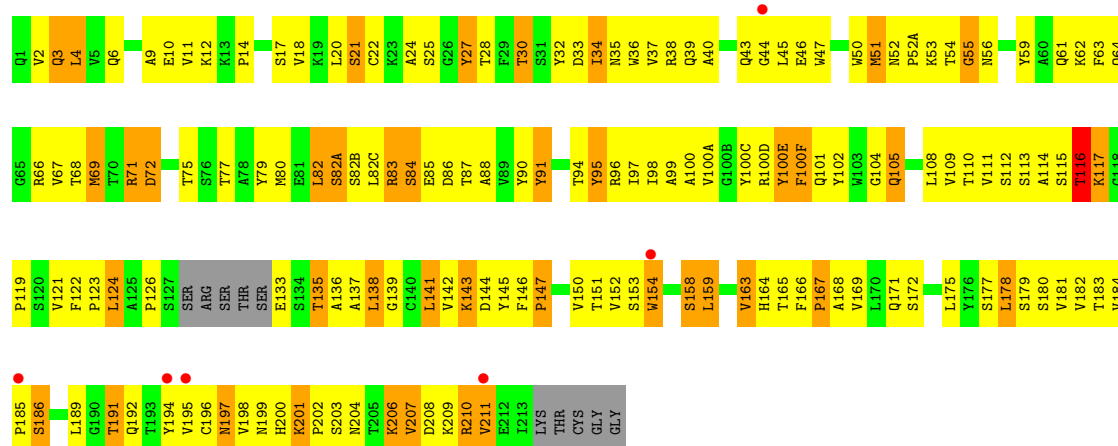




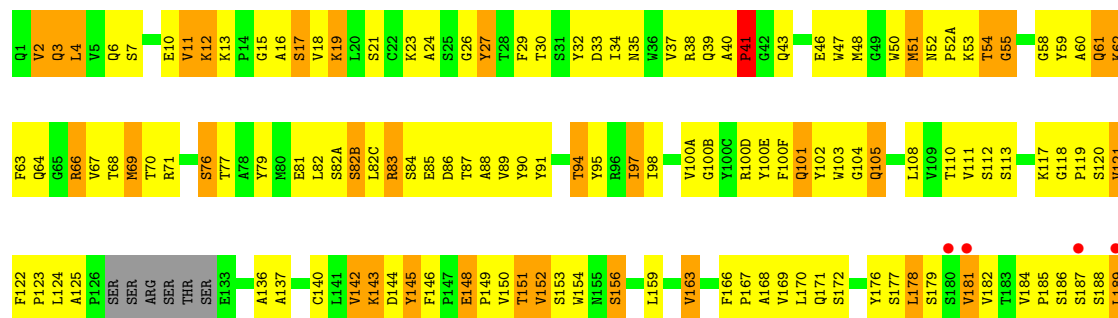
• Molecule 2: M48U1 CD4 MIMETIC PEPTIDE



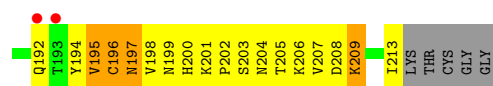
• Molecule 3: Rhesusized DH677.3 FAB HEAVY CHAIN



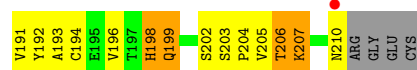
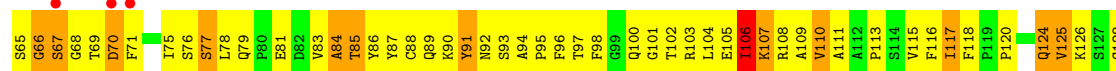
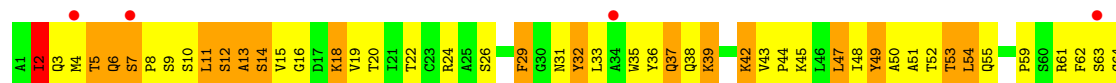
• Molecule 3: Rhesusized DH677.3 FAB HEAVY CHAIN



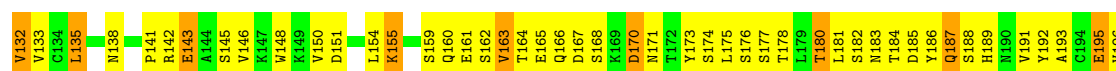
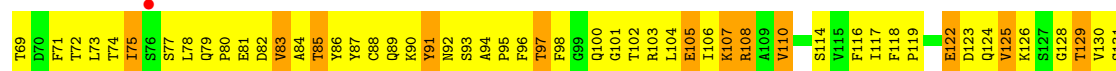
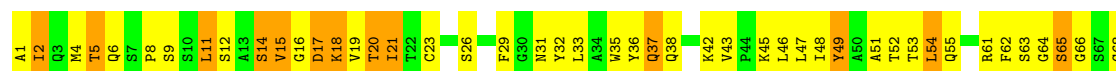




● Molecule 4: Rhesusized DH677.3 FAB LIGHT CHAIN



● Molecule 4: Rhesusized DH677.3 FAB LIGHT CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.18Å 82.66Å 111.90Å 90.00° 112.02° 90.00°	Depositor
Resolution (Å)	47.93 – 2.90 47.88 – 2.90	Depositor EDS
% Data completeness (in resolution range)	82.6 (47.93-2.90) 82.7 (47.88-2.90)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0258, PHENIX 1.17.1	Depositor
R, $R_{free}$	0.255 , 0.296 0.255 , 0.290	Depositor DCC
$R_{free}$ test set	1599 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.2	Xtriage
Anisotropy	0.640	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 50.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	12057	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NAG, NH2, U2X, MPT, DPR

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	0.62	0/2468	0.88	3/3346 (0.1%)
1	G	0.63	1/2702 (0.0%)	0.84	2/3667 (0.1%)
2	N	0.56	0/176	0.72	0/231
3	C	0.65	0/1691	0.83	0/2304
3	H	0.65	0/1697	0.87	1/2312 (0.0%)
4	D	0.67	0/1639	0.83	1/2231 (0.0%)
4	L	0.67	0/1639	0.89	2/2231 (0.1%)
All	All	0.64	1/12012 (0.0%)	0.86	9/16322 (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
2	N	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	124	GLY	C-N	8.12	1.47	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	392	ASN	N-CA-C	-7.93	89.58	111.00
4	L	32	TYR	N-CA-C	-7.14	91.72	111.00
4	L	32	TYR	CB-CA-C	-6.91	96.58	110.40
1	A	392	ASN	N-CA-CB	6.05	121.49	110.60
1	G	124	GLY	C-N-CA	-5.80	110.11	122.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	N	1	MPT	Mainchain

## 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	2419	0	2342	433	0
1	G	2646	0	2587	404	0
2	N	209	0	212	19	0
3	C	1651	0	1617	315	0
3	H	1657	0	1622	329	0
4	D	1604	0	1563	324	0
4	L	1604	0	1563	335	0
5	A	126	0	117	17	0
5	G	126	0	117	15	0
6	A	2	0	0	0	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
6	G	5	0	0	0	0
6	H	3	0	0	0	0
6	L	2	0	0	0	0
All	All	12057	0	11740	2030	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 85.

The worst 5 of 2030 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:G:259:LEU:HD12	1:G:374:HIS:CD2	1.31	1.58
3:H:163:VAL:CG2	3:H:182:VAL:HG13	1.31	1.57
3:C:87:THR:CG2	3:C:111:VAL:HG22	1.29	1.56
1:G:116:LEU:HD11	1:G:210:PHE:CE2	1.39	1.55
4:D:142:ARG:HB2	4:D:173:TYR:CD2	1.47	1.49

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	298/355 (84%)	224 (75%)	46 (15%)	28 (9%)	0	1
1	G	332/355 (94%)	272 (82%)	34 (10%)	26 (8%)	1	2
2	N	24/28 (86%)	20 (83%)	3 (12%)	1 (4%)	3	10
3	C	213/228 (93%)	173 (81%)	36 (17%)	4 (2%)	8	28
3	H	214/228 (94%)	176 (82%)	31 (14%)	7 (3%)	4	15
4	D	208/214 (97%)	175 (84%)	26 (12%)	7 (3%)	3	15
4	L	208/214 (97%)	159 (76%)	33 (16%)	16 (8%)	1	2
All	All	1497/1622 (92%)	1199 (80%)	209 (14%)	89 (6%)	1	5

5 of 89 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	240	LYS
1	G	248	THR
1	G	393	ASN
1	G	395	CYS
1	G	417	PRO

### 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	279/313 (89%)	202 (72%)	77 (28%)	0	1
1	G	302/313 (96%)	217 (72%)	85 (28%)	0	1
2	N	20/20 (100%)	19 (95%)	1 (5%)	24	57
3	C	183/192 (95%)	131 (72%)	52 (28%)	0	1
3	H	184/192 (96%)	135 (73%)	49 (27%)	0	1
4	D	184/187 (98%)	134 (73%)	50 (27%)	0	1
4	L	184/187 (98%)	133 (72%)	51 (28%)	0	1
All	All	1336/1404 (95%)	971 (73%)	365 (27%)	0	1

5 of 365 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	332	GLU
3	C	94	THR
1	A	360	ILE
1	A	488	VAL
3	C	152	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	192	GLN
4	D	31	ASN
4	D	187	GLN
3	H	197	ASN
3	H	192	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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
2	U2X	N	29	2	19,20,21	1.29	1 (5%)	22,25,27	1.56	5 (22%)

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
2	U2X	N	29	2	-	5/10/19/21	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	29	U2X	OH-CZ	3.69	1.46	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	29	U2X	CB-CG-CD2	-3.37	114.22	120.91
2	N	29	U2X	CG-CB-CA	2.85	119.86	114.10
2	N	29	U2X	C7-OH-CZ	-2.20	113.26	117.93
2	N	29	U2X	CB-CG-CD1	2.20	125.27	120.91
2	N	29	U2X	CE1-CD1-CG	-2.02	118.24	121.03

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	N	29	U2X	N-CA-CB-CG
2	N	29	U2X	CA-CB-CG-CD2
2	N	29	U2X	CA-CB-CG-CD1
2	N	29	U2X	C-CA-CB-CG
2	N	29	U2X	C4-C3-C7-OH

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	29	U2X	8	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

18 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	G	504	1	14,14,15	0.34	0	17,19,21	1.05	2 (11%)
5	NAG	A	505	1	14,14,15	0.28	0	17,19,21	1.70	3 (17%)
5	NAG	G	501	1	14,14,15	0.23	0	17,19,21	0.56	0
5	NAG	A	504	1	14,14,15	0.18	0	17,19,21	0.87	1 (5%)
5	NAG	A	509	1	14,14,15	0.49	0	17,19,21	0.86	1 (5%)
5	NAG	G	509	1	14,14,15	0.43	0	17,19,21	0.61	0
5	NAG	G	505	1	14,14,15	1.38	1 (7%)	17,19,21	1.80	2 (11%)
5	NAG	G	503	1	14,14,15	0.30	0	17,19,21	0.60	0
5	NAG	G	507	1	14,14,15	0.26	0	17,19,21	0.38	0
5	NAG	A	508	1	14,14,15	0.22	0	17,19,21	0.90	1 (5%)
5	NAG	A	507	1	14,14,15	0.24	0	17,19,21	0.45	0
5	NAG	A	502	1	14,14,15	0.70	1 (7%)	17,19,21	1.85	1 (5%)
5	NAG	G	502	1	14,14,15	0.40	0	17,19,21	1.52	1 (5%)
5	NAG	A	501	1	14,14,15	0.35	0	17,19,21	0.62	0
5	NAG	G	506	1	14,14,15	0.91	1 (7%)	17,19,21	1.20	2 (11%)
5	NAG	A	506	1	14,14,15	0.41	0	17,19,21	0.71	0
5	NAG	A	503	1	14,14,15	0.44	0	17,19,21	0.79	1 (5%)
5	NAG	G	508	1	14,14,15	0.28	0	17,19,21	0.67	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	G	504	1	-	0/6/23/26	0/1/1/1
5	NAG	A	505	1	-	5/6/23/26	0/1/1/1
5	NAG	G	501	1	-	0/6/23/26	0/1/1/1
5	NAG	A	504	1	-	0/6/23/26	0/1/1/1
5	NAG	A	509	1	-	2/6/23/26	0/1/1/1
5	NAG	G	509	1	-	2/6/23/26	0/1/1/1
5	NAG	G	505	1	-	2/6/23/26	0/1/1/1
5	NAG	G	503	1	-	0/6/23/26	0/1/1/1
5	NAG	G	507	1	-	2/6/23/26	0/1/1/1
5	NAG	A	508	1	-	2/6/23/26	0/1/1/1
5	NAG	A	507	1	-	0/6/23/26	0/1/1/1
5	NAG	A	502	1	-	2/6/23/26	0/1/1/1
5	NAG	G	502	1	-	2/6/23/26	0/1/1/1
5	NAG	A	501	1	-	2/6/23/26	0/1/1/1
5	NAG	G	506	1	-	0/6/23/26	0/1/1/1
5	NAG	A	506	1	-	2/6/23/26	0/1/1/1
5	NAG	A	503	1	-	2/6/23/26	0/1/1/1
5	NAG	G	508	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	505	NAG	O5-C1	4.19	1.50	1.43
5	G	506	NAG	O5-C1	-2.97	1.39	1.43
5	A	502	NAG	O5-C1	2.32	1.47	1.43

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	502	NAG	C1-O5-C5	7.37	122.17	112.19
5	G	502	NAG	C1-O5-C5	5.86	120.13	112.19
5	G	505	NAG	O5-C1-C2	-5.63	102.39	111.29
5	A	505	NAG	C2-N2-C7	4.31	129.04	122.90
5	A	508	NAG	C1-O5-C5	3.34	116.71	112.19

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	509	NAG	C8-C7-N2-C2
5	A	509	NAG	O7-C7-N2-C2
5	A	501	NAG	O5-C5-C6-O6
5	G	502	NAG	O5-C5-C6-O6
5	A	506	NAG	O5-C5-C6-O6

There are no ring outliers.

12 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	504	NAG	1	0
5	A	505	NAG	4	0
5	A	509	NAG	4	0
5	G	505	NAG	6	0
5	G	503	NAG	1	0
5	A	508	NAG	2	0
5	A	507	NAG	2	0
5	A	502	NAG	2	0
5	G	506	NAG	6	0
5	A	506	NAG	2	0
5	A	503	NAG	1	0
5	G	508	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	308/355 (86%)	0.17	10 (3%) 47 43	44, 80, 126, 169	0
1	G	338/355 (95%)	-0.13	6 (1%) 68 67	31, 68, 102, 119	0
2	N	24/28 (85%)	0.13	1 (4%) 36 32	37, 56, 80, 98	0
3	C	217/228 (95%)	-0.03	6 (2%) 53 49	36, 63, 88, 116	0
3	H	218/228 (95%)	0.01	6 (2%) 53 49	48, 70, 99, 116	0
4	D	210/214 (98%)	-0.14	1 (0%) 91 91	36, 60, 79, 95	0
4	L	210/214 (98%)	0.06	8 (3%) 40 36	51, 69, 90, 111	0
All	All	1525/1622 (94%)	-0.01	38 (2%) 57 55	31, 68, 106, 169	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	189	LEU	5.4
1	A	118	PRO	4.4
1	A	367	GLY	4.3
1	A	71	THR	4.0
3	H	194	TYR	3.9

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
2	DPR	N	21	7/8	0.92	0.27	47,51,61,75	0
2	U2X	N	29	19/20	0.94	0.18	25,30,52,53	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
5	NAG	G	509	14/15	0.74	0.41	65,81,89,94	0
5	NAG	A	509	14/15	0.77	0.21	86,92,102,103	0
5	NAG	G	506	14/15	0.80	0.26	76,85,97,97	0
5	NAG	G	502	14/15	0.81	0.22	69,74,80,84	0
5	NAG	A	505	14/15	0.84	0.26	50,63,79,86	0
5	NAG	G	504	14/15	0.85	0.23	96,106,115,116	0
5	NAG	G	505	14/15	0.85	0.18	27,33,37,37	0
5	NAG	A	507	14/15	0.86	0.23	60,75,89,99	0
5	NAG	A	504	14/15	0.87	0.26	66,73,86,93	0
5	NAG	G	508	14/15	0.88	0.18	60,64,72,80	0
5	NAG	A	506	14/15	0.88	0.23	62,72,77,85	0
5	NAG	A	508	14/15	0.89	0.26	70,82,101,101	0
5	NAG	G	507	14/15	0.90	0.17	58,65,92,92	0
5	NAG	A	502	14/15	0.90	0.18	70,76,82,83	0
5	NAG	A	501	14/15	0.91	0.19	47,52,66,80	0
5	NAG	G	501	14/15	0.92	0.16	44,57,69,70	0
5	NAG	G	503	14/15	0.95	0.18	44,54,68,75	0
5	NAG	A	503	14/15	0.95	0.15	39,43,56,59	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.