



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:00 am GMT

PDB ID : 4DJ7  
Title : Structure of the hemagglutinin complexed with 3SLN from a highly pathogenic H7N7 influenza virus  
Authors : Yang, H.; Carney, P.J.; Donis, R.O.; Stevens, J.  
Deposited on : 2012-02-01  
Resolution : 2.81 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (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

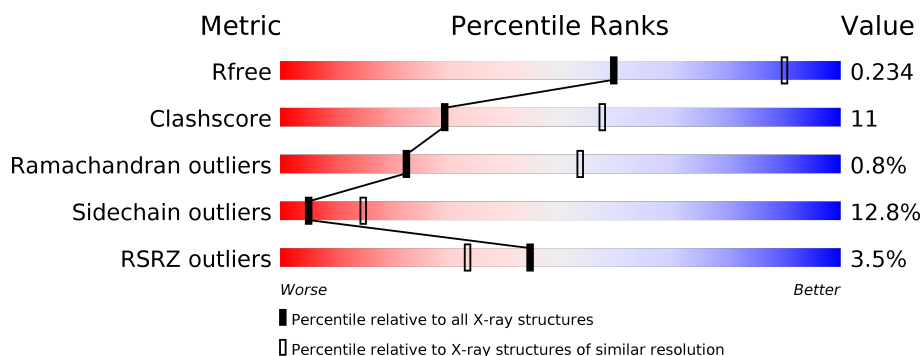
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.81 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	2917 (2.84-2.80)
Clashscore	112137	3382 (2.84-2.80)
Ramachandran outliers	110173	3324 (2.84-2.80)
Sidechain outliers	110143	3326 (2.84-2.80)
RSRZ outliers	101464	2948 (2.84-2.80)

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  $\geq 3$ , 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	327	<div> <div>73%</div> <div>19%</div> <div>• •</div> </div>
1	C	327	<div>2%</div> <div>72%</div> <div>20%</div> <div>• •</div>
1	E	327	<div>%</div> <div>76%</div> <div>18%</div> <div>• •</div>
2	B	177	<div>6%</div> <div>65%</div> <div>25%</div> <div>6%</div> <div>• •</div>
2	D	177	<div>7%</div> <div>67%</div> <div>23%</div> <div>5%</div> <div>• •</div>
2	F	177	<div>9%</div> <div>62%</div> <div>28%</div> <div>5%</div> <div>5%</div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	404	X	-	-	-
4	NAG	B	201	X	-	-	-
4	NAG	C	403	X	-	-	-
4	NAG	E	403	X	-	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11749 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	6	0	0
			2422	1502	435	471	14			
1	C	315	Total	C	N	O	S	0	0	0
			2414	1498	434	468	14			
1	E	317	Total	C	N	O	S	4	0	0
			2426	1504	436	472	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ALA	-	EXPRESSION TAG	UNP Q6VMK1
A	-2	ASP	-	EXPRESSION TAG	UNP Q6VMK1
A	-1	PRO	-	EXPRESSION TAG	UNP Q6VMK1
A	0	GLY	-	EXPRESSION TAG	UNP Q6VMK1
C	-3	ALA	-	EXPRESSION TAG	UNP Q6VMK1
C	-2	ASP	-	EXPRESSION TAG	UNP Q6VMK1
C	-1	PRO	-	EXPRESSION TAG	UNP Q6VMK1
C	0	GLY	-	EXPRESSION TAG	UNP Q6VMK1
E	-3	ALA	-	EXPRESSION TAG	UNP Q6VMK1
E	-2	ASP	-	EXPRESSION TAG	UNP Q6VMK1
E	-1	PRO	-	EXPRESSION TAG	UNP Q6VMK1
E	0	GLY	-	EXPRESSION TAG	UNP Q6VMK1

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	170	Total	C	N	O	S	4	0	0
			1380	851	243	279	7			
2	D	171	Total	C	N	O	S	0	0	0
			1388	857	244	280	7			
2	F	169	Total	C	N	O	S	0	0	0
			1369	845	239	278	7			

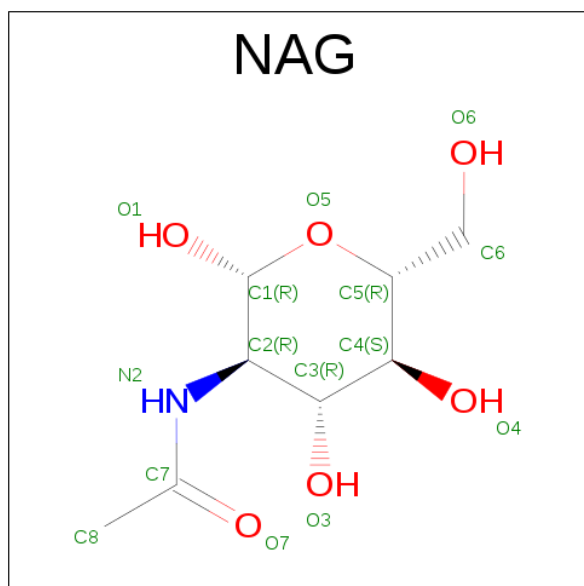
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	EXPRESSION TAG	UNP Q6VMK1
B	176	GLY	-	EXPRESSION TAG	UNP Q6VMK1
B	177	ARG	-	EXPRESSION TAG	UNP Q6VMK1
D	175	SER	-	EXPRESSION TAG	UNP Q6VMK1
D	176	GLY	-	EXPRESSION TAG	UNP Q6VMK1
D	177	ARG	-	EXPRESSION TAG	UNP Q6VMK1
F	175	SER	-	EXPRESSION TAG	UNP Q6VMK1
F	176	GLY	-	EXPRESSION TAG	UNP Q6VMK1
F	177	ARG	-	EXPRESSION TAG	UNP Q6VMK1

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	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
			46	25	2	19		
5	C	3	Total	C	N	O	0	0
			46	25	2	19		
5	E	3	Total	C	N	O	0	0
			46	25	2	19		

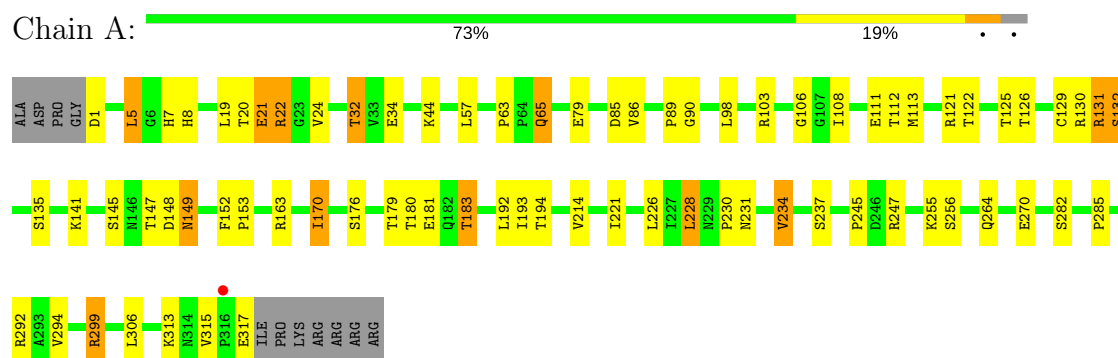
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	O	0	0
			3	3		
6	B	4	Total	O	0	0
			4	4		
6	C	7	Total	O	0	0
			7	7		
6	D	5	Total	O	0	0
			5	5		
6	E	6	Total	O	0	0
			6	6		
6	F	5	Total	O	0	0
			5	5		

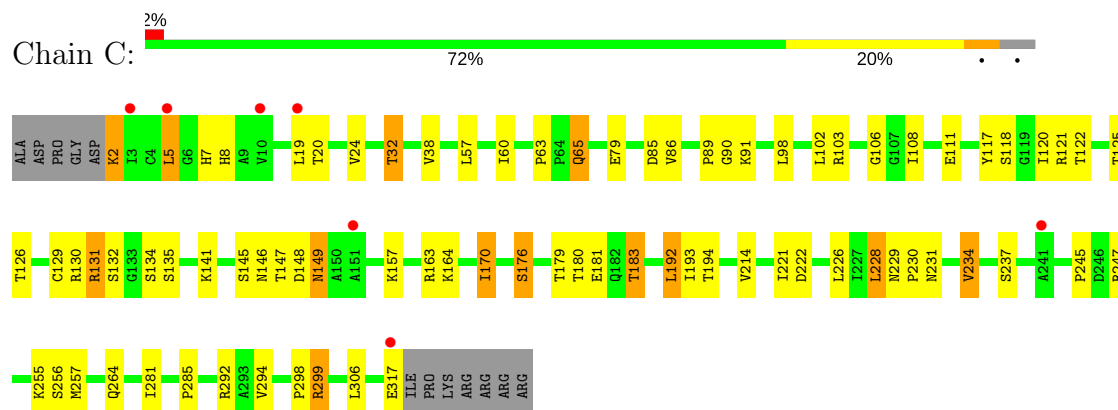
### 3 Residue-property plots [i](#)

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.

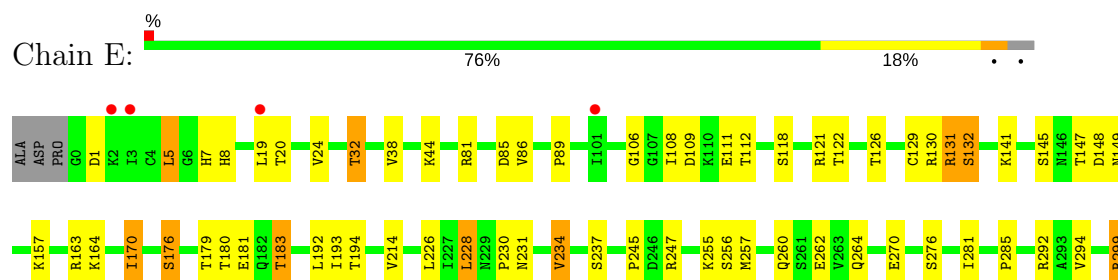
#### • Molecule 1: Hemagglutinin



#### • Molecule 1: Hemagglutinin

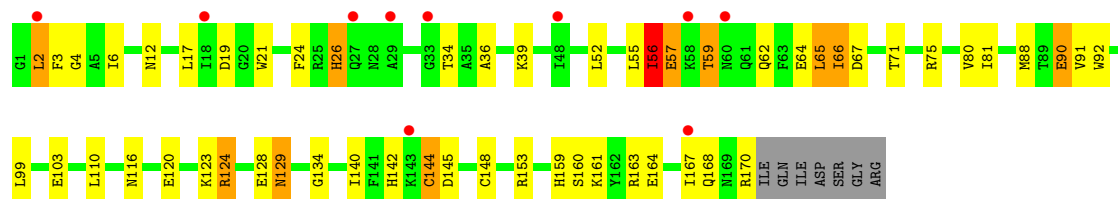


#### • Molecule 1: Hemagglutinin

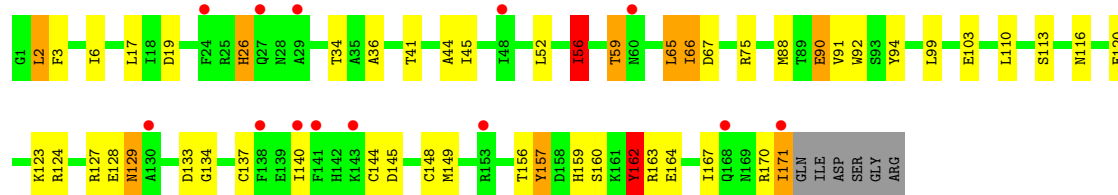




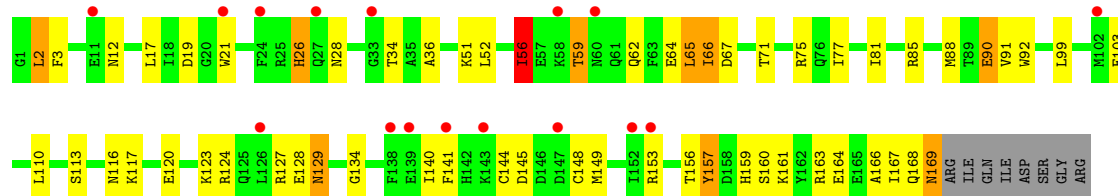
• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	200.28Å 115.72Å 117.66Å 90.00° 124.39° 90.00°	Depositor
Resolution (Å)	50.00 – 2.81 41.32 – 2.81	Depositor EDS
% Data completeness (in resolution range)	97.2 (50.00-2.81) 96.7 (41.32-2.81)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.207 , 0.243 0.205 , 0.234	Depositor DCC
$R_{free}$ test set	2681 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	85.3	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 52.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for $1/2^*h+1/2^*k+2^*l, 1/2^*h+1/2^*k, -1/2^*h+1/2^*k-l$ 0.004 for $-1/2^*h-3/2^*k-l, -1/2^*h+1/2^*k-l, 1/2^*h+1/2^*k$ 0.005 for $-1/2^*h+3/2^*k-l, 1/2^*h+1/2^*k+l, 1/2^*h-1/2^*k$ 0.010 for $1/2^*h-1/2^*k+2^*l, -1/2^*h+1/2^*k, -1/2^*h-1/2^*k-l$ 0.013 for $-h+k-l, -l, -k$ 0.000 for $-h-k-l, l, k$ 0.009 for $-1/2^*h+1/2^*k+l, 1/2^*h-1/2^*k+l, 1/2^*h+1/2^*k$ 0.006 for $-1/2^*h-1/2^*k+l, -1/2^*h-1/2^*k-l, 1/2^*h-1/2^*k$ 0.419 for $1/2^*h+3/2^*k, 1/2^*h-1/2^*k, -1/2^*h-1/2^*k-l$ 0.407 for $1/2^*h-3/2^*k, -1/2^*h-1/2^*k, -1/2^*h+1/2^*k-l$ 0.012 for $-h-2^*l, -k, l$	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11749	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	103.0	wwPDB-VP

<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.

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% of the height of the origin peak. No significant pseudotranslation is detected.*

## 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: SIA, GAL, 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	0.75	2/2468 (0.1%)	2.32	4/3337 (0.1%)
1	C	0.49	1/2460 (0.0%)	0.59	0/3326
1	E	0.47	0/2472	0.65	2/3342 (0.1%)
2	B	0.54	1/1404 (0.1%)	0.52	0/1892
2	D	0.49	1/1412 (0.1%)	0.52	0/1903
2	F	0.56	0/1393	0.54	0/1878
All	All	0.56	5/11609 (0.0%)	1.19	6/15678 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	C	0	1
1	E	0	1
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	21	GLU	CG-CD	-23.36	1.17	1.51
1	A	22	ARG	NE-CZ	-16.84	1.11	1.33
2	B	39	LYS	CB-CG	-10.79	1.23	1.52
1	C	2	LYS	C-O	6.37	1.35	1.23
2	D	162	TYR	CG-CD2	-5.42	1.32	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	ARG	NE-CZ-NH1	-122.46	59.07	120.30
1	A	22	ARG	CD-NE-CZ	-35.88	73.37	123.60
1	A	22	ARG	NE-CZ-NH2	17.58	129.09	120.30
1	E	164	LYS	CA-CB-CG	-16.70	76.66	113.40
1	A	21	GLU	CG-CD-OE1	-15.49	87.32	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	GLU	Sidechain
1	A	22	ARG	Sidechain
1	A	85	ASP	Peptide
1	C	85	ASP	Peptide
1	E	85	ASP	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	2422	0	2369	43	0
1	C	2414	0	2362	48	0
1	E	2426	0	2372	40	0
2	B	1380	0	1283	50	0
2	D	1388	0	1294	42	0
2	F	1369	0	1270	48	0
3	A	28	0	25	2	0
4	A	28	0	26	0	0
4	B	14	0	13	3	0
4	C	42	0	39	1	0
4	D	14	0	13	2	0
4	E	42	0	39	0	0
4	F	14	0	13	2	0
5	A	46	0	40	5	0
5	C	46	0	40	5	0
5	E	46	0	40	7	0
6	A	3	0	0	0	0
6	B	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	7	0	0	0	0
6	D	5	0	0	0	0
6	E	6	0	0	1	0
6	F	5	0	0	0	0
All	All	11749	0	11238	248	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 11.

The worst 5 of 248 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)
5:C:404:SIA:H113	5:C:404:SIA:O7	1.43	1.18
5:A:405:SIA:O7	5:A:405:SIA:H113	1.46	1.14
5:E:404:SIA:H113	5:E:404:SIA:O7	1.45	1.11
2:D:128:GLU:HG3	2:D:170:ARG:HH12	1.17	1.08
5:E:404:SIA:HO7	5:E:404:SIA:H113	1.25	0.97

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	314/327 (96%)	295 (94%)	17 (5%)	2 (1%)	28	61
1	C	313/327 (96%)	294 (94%)	18 (6%)	1 (0%)	44	76
1	E	315/327 (96%)	296 (94%)	18 (6%)	1 (0%)	44	76
2	B	168/177 (95%)	153 (91%)	14 (8%)	1 (1%)	28	61
2	D	169/177 (96%)	151 (89%)	15 (9%)	3 (2%)	10	30
2	F	167/177 (94%)	152 (91%)	11 (7%)	4 (2%)	7	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1446/1512 (96%)	1341 (93%)	93 (6%)	12 (1%)	22 53

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	SER
1	E	132	SER
1	A	149	ASN
2	B	56	ILE
1	C	149	ASN

### 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	268/277 (97%)	237 (88%)	31 (12%)	6 19
1	C	267/277 (96%)	231 (86%)	36 (14%)	4 13
1	E	268/277 (97%)	236 (88%)	32 (12%)	6 17
2	B	145/151 (96%)	124 (86%)	21 (14%)	4 11
2	D	146/151 (97%)	128 (88%)	18 (12%)	5 16
2	F	144/151 (95%)	123 (85%)	21 (15%)	3 10
All	All	1238/1284 (96%)	1079 (87%)	159 (13%)	5 15

5 of 159 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	164	LYS
2	D	19	ASP
2	F	65	LEU
1	C	180	THR
1	C	237	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

11 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	$\# Z  > 2$
3	NAG	A	401	1,3	14,14,15	0.48	0	15,19,21	1.14	1 (6%)
3	NAG	A	402	3	14,14,15	0.65	0	15,19,21	1.30	1 (6%)
5	SIA	A	405	5	17,20,21	0.28	0	19,28,31	1.20	1 (5%)
5	NAG	A	406	5	15,15,15	0.43	0	21,21,21	1.05	3 (14%)
5	GAL	A	407	5	11,11,12	0.66	0	13,15,17	0.85	1 (7%)
5	SIA	C	404	5	17,20,21	0.26	0	19,28,31	0.93	0
5	NAG	C	405	5	15,15,15	0.41	0	21,21,21	1.05	1 (4%)
5	GAL	C	406	5	11,11,12	0.67	0	13,15,17	0.79	0
5	SIA	E	404	5	17,20,21	0.28	0	19,28,31	0.73	0
5	NAG	E	405	5	15,15,15	0.45	0	21,21,21	1.11	3 (14%)
5	GAL	E	406	5	11,11,12	0.69	0	13,15,17	0.88	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	401	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	402	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SIA	A	405	5	-	0/14/34/38	0/1/1/1
5	NAG	A	406	5	-	0/6/26/26	0/1/1/1
5	GAL	A	407	5	-	0/2/19/22	0/1/1/1
5	SIA	C	404	5	-	0/14/34/38	0/1/1/1
5	NAG	C	405	5	-	0/6/26/26	0/1/1/1
5	GAL	C	406	5	-	0/2/19/22	0/1/1/1
5	SIA	E	404	5	-	0/14/34/38	0/1/1/1
5	NAG	E	405	5	-	0/6/26/26	0/1/1/1
5	GAL	E	406	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	NAG	C3-C4-C5	-3.82	103.48	110.22
5	A	405	SIA	C3-C4-C5	-3.09	107.73	111.46
5	A	406	NAG	C4-C3-C2	2.19	113.58	110.33
5	E	405	NAG	C3-C4-C5	2.20	114.08	110.22
5	A	406	NAG	C3-C4-C5	2.22	114.14	110.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	NAG	2	0
3	A	402	NAG	2	0
5	A	405	SIA	5	0
5	A	407	GAL	1	0
5	C	404	SIA	5	0
5	E	404	SIA	7	0
5	E	406	GAL	1	0

## 5.6 Ligand geometry ⓘ

11 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	$\# Z  > 2$
4	NAG	A	403	1	14,14,15	0.49	0	15,19,21	1.17	1 (6%)
4	NAG	A	404	1	14,14,15	0.72	0	15,19,21	1.44	2 (13%)
4	NAG	B	201	2	14,14,15	0.35	0	15,19,21	1.28	2 (13%)
4	NAG	C	401	1	14,14,15	0.51	0	15,19,21	0.92	1 (6%)
4	NAG	C	402	1	14,14,15	0.47	0	15,19,21	1.40	1 (6%)
4	NAG	C	403	1	14,14,15	0.50	0	15,19,21	0.87	1 (6%)
4	NAG	D	201	2	14,14,15	0.51	0	15,19,21	1.58	1 (6%)
4	NAG	E	401	1	14,14,15	0.52	0	15,19,21	0.82	0
4	NAG	E	402	1	14,14,15	0.50	0	15,19,21	1.20	1 (6%)
4	NAG	E	403	1	14,14,15	0.44	0	15,19,21	0.75	0
4	NAG	F	201	2	14,14,15	0.45	0	15,19,21	1.21	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	403	1	-	0/6/23/26	0/1/1/1
4	NAG	A	404	1	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	B	201	2	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	C	401	1	-	0/6/23/26	0/1/1/1
4	NAG	C	402	1	-	0/6/23/26	0/1/1/1
4	NAG	C	403	1	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	D	201	2	-	0/6/23/26	0/1/1/1
4	NAG	E	401	1	-	0/6/23/26	0/1/1/1
4	NAG	E	402	1	-	0/6/23/26	0/1/1/1
4	NAG	E	403	1	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	F	201	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	401	NAG	C3-C4-C5	-2.74	105.39	110.22
4	B	201	NAG	C4-C3-C2	-2.64	107.16	111.02
4	A	404	NAG	C4-C3-C2	2.28	114.35	111.02
4	C	403	NAG	O5-C1-C2	2.60	115.09	111.47
4	B	201	NAG	C1-O5-C5	3.25	116.65	112.17

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	403	NAG	C1
4	E	403	NAG	C1
4	B	201	NAG	C1
4	A	404	NAG	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	201	NAG	3	0
4	C	403	NAG	1	0
4	D	201	NAG	2	0
4	F	201	NAG	2	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	316/327 (96%)	0.14	1 (0%) 93 92	58, 86, 121, 153	2 (0%)
1	C	315/327 (96%)	0.21	7 (2%) 62 52	61, 89, 125, 146	0
1	E	317/327 (96%)	0.20	4 (1%) 77 71	60, 87, 120, 168	1 (0%)
2	B	170/177 (96%)	0.45	10 (5%) 23 15	53, 116, 180, 185	1 (0%)
2	D	171/177 (96%)	0.51	13 (7%) 15 8	53, 117, 185, 191	0
2	F	169/177 (95%)	0.54	16 (9%) 9 5	54, 119, 186, 192	0
All	All	1458/1512 (96%)	0.30	51 (3%) 44 33	53, 93, 176, 192	4 (0%)

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	143	LYS	5.3
2	D	143	LYS	4.4
2	B	29	ALA	4.1
2	B	60	ASN	4.1
2	F	141	PHE	4.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SIA	E	404	20/21	0.92	0.28	1.22	124,144,163,166	0
5	SIA	C	404	20/21	0.94	0.20	0.01	126,154,177,179	0
5	SIA	A	405	20/21	0.93	0.21	-0.07	117,142,168,172	0
5	GAL	C	406	11/12	0.81	0.16	-	169,188,201,208	0
5	GAL	E	406	11/12	0.87	0.17	-	157,175,185,192	0
5	NAG	A	406	15/15	0.82	0.17	-	207,226,231,235	0
5	GAL	A	407	11/12	0.84	0.18	-	166,176,184,189	0
3	NAG	A	401	14/15	0.78	0.20	-	167,187,214,229	0
5	NAG	E	405	15/15	0.76	0.20	-	185,222,233,235	0
5	NAG	C	405	15/15	0.79	0.18	-	222,238,242,245	0
3	NAG	A	402	14/15	0.82	0.20	-	233,241,247,248	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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	D	201	14/15	0.80	0.17	-0.15	126,149,165,171	0
4	NAG	B	201	14/15	0.81	0.18	-0.33	129,153,163,170	0
4	NAG	F	201	14/15	0.88	0.16	-0.75	132,156,164,171	0
4	NAG	E	403	14/15	0.79	0.20	-	190,209,223,228	0
4	NAG	E	402	14/15	0.81	0.22	-	152,170,177,179	0
4	NAG	C	401	14/15	0.83	0.23	-	159,176,196,199	0
4	NAG	A	403	14/15	0.71	0.29	-	156,174,183,184	0
4	NAG	C	403	14/15	0.68	0.26	-	186,198,221,221	0
4	NAG	C	402	14/15	0.82	0.27	-	147,168,196,201	0
4	NAG	E	401	14/15	0.86	0.20	-	151,173,189,191	0
4	NAG	A	404	14/15	0.55	0.28	-	167,200,217,221	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.