



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2018 – 11:18 PM EST

PDB ID : 6BKQ  
Title : Crystal structure of the A/Hong Kong/1/1968 (H3N2) influenza virus hemagglutinin E190D mutant in complex with 6'-SLN  
Authors : Wu, N.C.; Wilson, I.A.  
Deposited on : 2017-11-09  
Resolution : 2.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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 : rb-20030736  
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) : rb-20030736

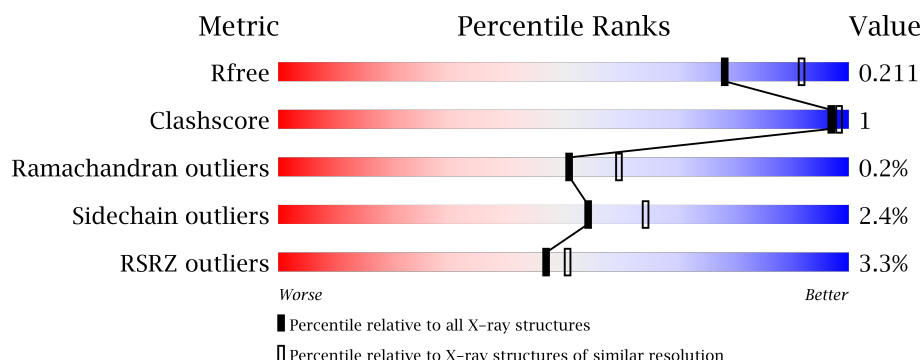
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1062 (2.26-2.26)
Clashscore	112137	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)
RSRZ outliers	101464	1066 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	323	<div> <div>4%</div> <div>92%</div> <div>7%</div> <div>..</div> </div>
1	C	323	<div> <div>%</div> <div>94%</div> <div>..</div> </div>
1	E	323	<div> <div>%</div> <div>95%</div> <div>..</div> </div>
2	B	174	<div> <div>7%</div> <div>97%</div> <div>..</div> </div>
2	D	174	<div> <div>4%</div> <div>95%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	174	

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
3	NAG	A	408	-	-	-	X
3	NAG	E	501	-	-	-	X
3	NAG	E	507	-	-	-	X
8	TAM	C	510	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12808 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	321	Total	C	N	O	S	0	0	0
			2478	1551	438	476	13			
1	C	317	Total	C	N	O	S	0	0	0
			2442	1530	429	470	13			
1	E	317	Total	C	N	O	S	0	0	0
			2442	1530	429	470	13			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP Q91MA7
A	8	ASP	-	expression tag	UNP Q91MA7
A	9	PRO	-	expression tag	UNP Q91MA7
A	10	GLY	-	expression tag	UNP Q91MA7
A	190	ASP	GLU	engineered mutation	UNP Q91MA7
C	7	ALA	-	expression tag	UNP Q91MA7
C	8	ASP	-	expression tag	UNP Q91MA7
C	9	PRO	-	expression tag	UNP Q91MA7
C	10	GLY	-	expression tag	UNP Q91MA7
C	190	ASP	GLU	engineered mutation	UNP Q91MA7
E	7	ALA	-	expression tag	UNP Q91MA7
E	8	ASP	-	expression tag	UNP Q91MA7
E	9	PRO	-	expression tag	UNP Q91MA7
E	10	GLY	-	expression tag	UNP Q91MA7
E	190	ASP	GLU	engineered mutation	UNP Q91MA7

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1391	863	243	279	6			

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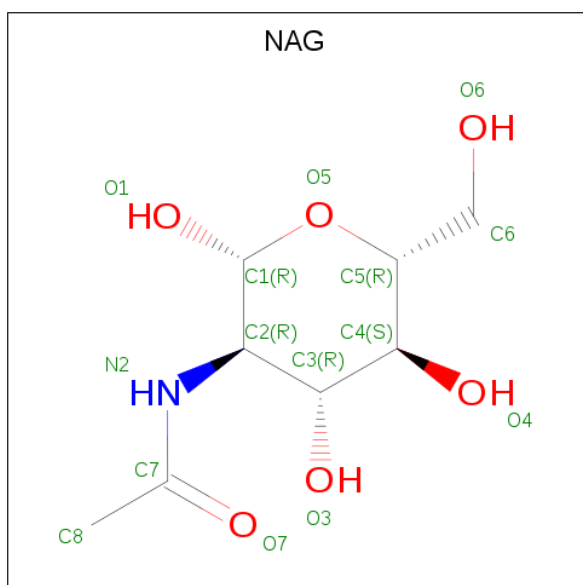
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	171	Total	C	N	O	S	0	0	0
			1382	858	241	277	6			
2	F	171	Total	C	N	O	S	0	0	0
			1382	858	241	277	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	123	GLY	ARG	conflict	UNP Q91MA7
D	123	GLY	ARG	conflict	UNP Q91MA7
F	123	GLY	ARG	conflict	UNP Q91MA7

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



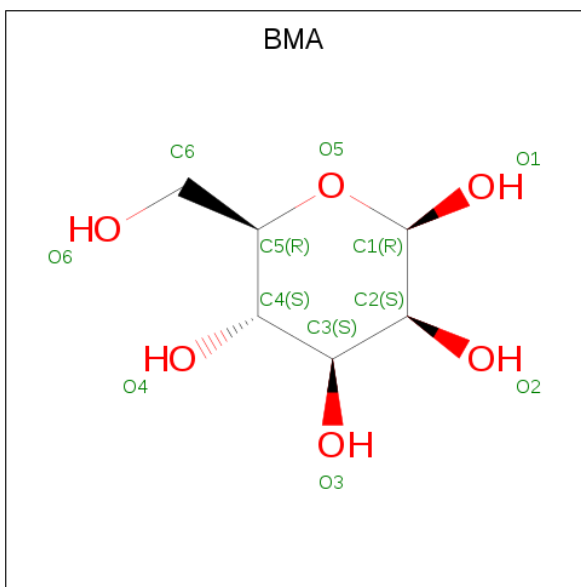
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O		0	0
			14	8	1	5			
3	A	1	Total	C	N	O		0	0
			14	8	1	5			
3	A	1	Total	C	N	O		0	0
			14	8	1	5			
3	A	1	Total	C	N	O		0	0
			14	8	1	5			
3	A	1	Total	C	N	O		0	0
			14	8	1	5			

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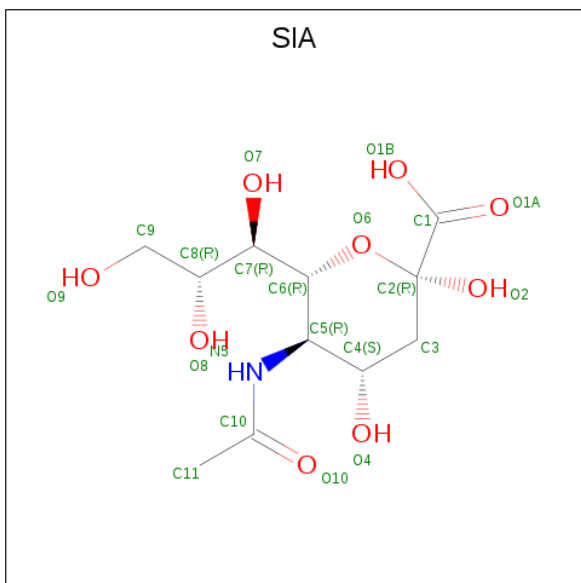
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			15	8	1	6		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			15	8	1	6		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



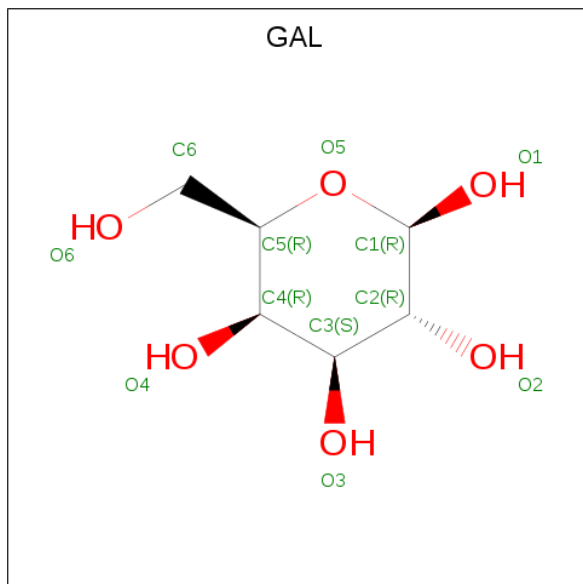
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	E	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is O-SIALIC ACID (three-letter code: SIA) (formula:  $C_{11}H_{19}NO_9$ ).



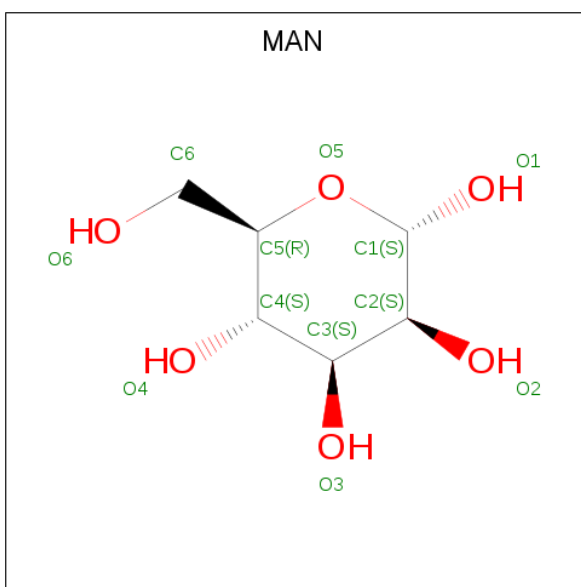
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			20	11	1	8		
5	C	1	Total	C	N	O	0	0
			20	11	1	8		
5	E	1	Total	C	N	O	0	0
			20	11	1	8		

- Molecule 6 is BETA-D-GALACTOSE (three-letter code: GAL) (formula:  $C_6H_{12}O_6$ ).



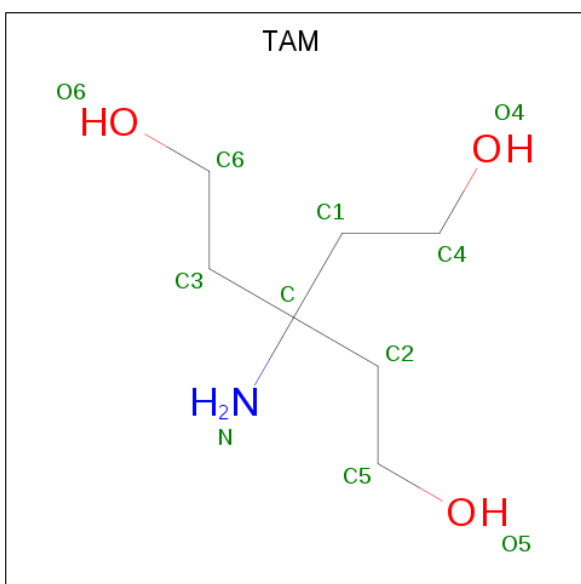
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	C	1	Total	C	O	0	0
			11	6	5		
6	E	1	Total	C	O	0	0
			12	6	6		

- Molecule 7 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			11	6	5		
7	C	1	Total	C	O	0	0
			11	6	5		
7	E	1	Total	C	O	0	0
			11	6	5		
7	E	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula:  $C_7H_{17}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			11	7	1	3		
8	E	1	Total	C	N	O	0	0
			11	7	1	3		

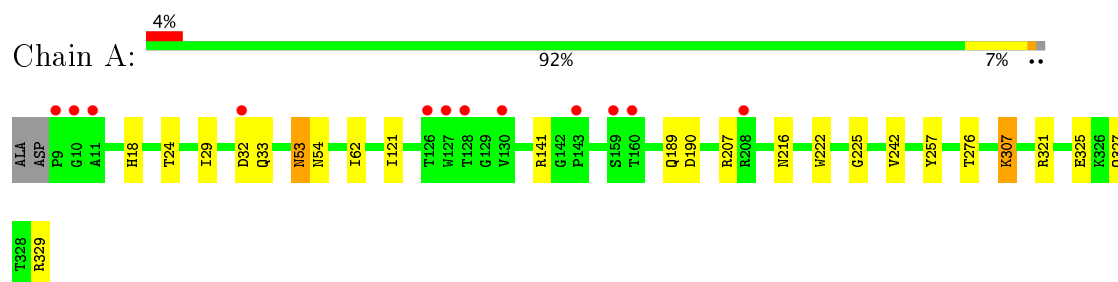
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	162	Total	O	0	0
			162	162		
9	B	91	Total	O	0	0
			91	91		
9	C	158	Total	O	0	0
			158	158		
9	D	89	Total	O	0	0
			89	89		
9	E	205	Total	O	0	0
			205	205		
9	F	100	Total	O	0	0
			100	100		

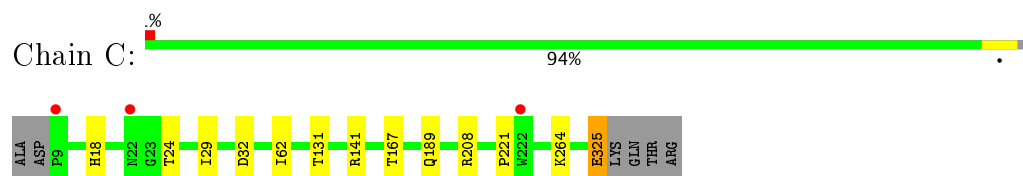
### 3 Residue-property plots [i](#)

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.

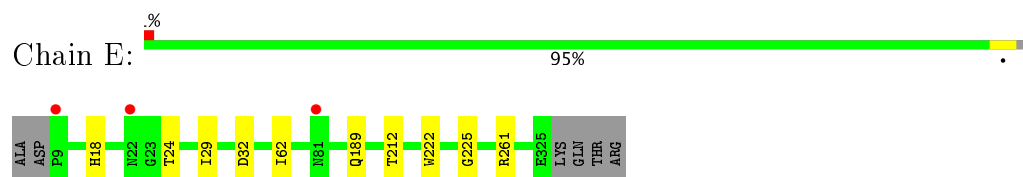
#### • Molecule 1: Hemagglutinin



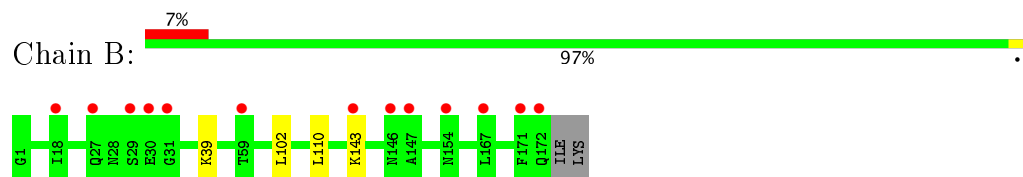
#### • Molecule 1: Hemagglutinin



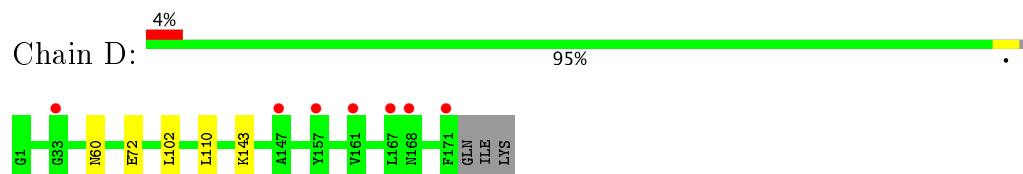
#### • Molecule 1: Hemagglutinin



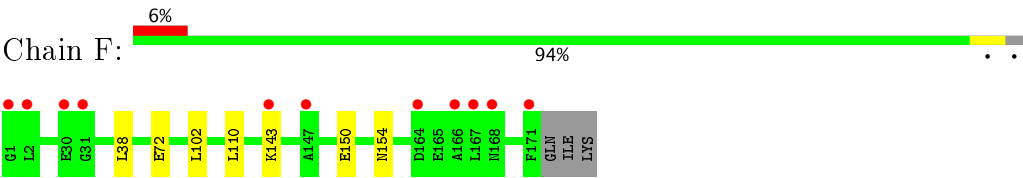
#### • Molecule 2: Hemagglutinin



#### • 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, $\alpha$ , $\beta$ , $\gamma$	208.78 Å   130.84 Å   72.18 Å 90.00°   97.90°   90.00°	Depositor
Resolution (Å)	50.00 – 2.25 49.46 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.25) 99.2 (49.46-2.24)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 2.25 Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.178   ,   0.208 0.182   ,   0.211	Depositor DCC
$R_{free}$ test set	4549 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.9	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 41.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12808	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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: BMA, NAG, SIA, GAL, TAM, MAN

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	0.51	0/2535	0.71	0/3453
1	C	0.51	0/2499	0.73	0/3406
1	E	0.54	0/2499	0.72	0/3406
2	B	0.47	0/1415	0.66	0/1902
2	D	0.47	0/1406	0.67	0/1890
2	F	0.47	0/1406	0.69	0/1890
All	All	0.50	0/11760	0.70	0/15947

There are no bond length outliers.

There are no bond angle outliers.

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	2478	0	2429	16	0
1	C	2442	0	2388	6	0
1	E	2442	0	2389	5	0
2	B	1391	0	1307	1	0
2	D	1382	0	1299	1	0
2	F	1382	0	1299	2	0
3	A	113	0	100	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	99	0	89	0	0
3	E	70	0	62	0	0
4	A	22	0	20	0	0
4	C	11	0	8	0	0
4	E	11	0	8	0	0
5	A	20	0	17	0	0
5	C	20	0	17	0	0
5	E	20	0	17	0	0
6	A	11	0	9	0	0
6	C	11	0	9	0	0
6	E	12	0	11	0	0
7	C	22	0	20	0	0
7	E	22	0	20	0	0
8	C	11	0	17	1	0
8	E	11	0	17	0	0
9	A	162	0	0	3	0
9	B	91	0	0	0	0
9	C	158	0	0	0	0
9	D	89	0	0	0	0
9	E	205	0	0	1	0
9	F	100	0	0	0	0
All	All	12808	0	11552	26	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 1.

All (26) 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:E:261:ARG:NH2	9:E:601:HOH:O	2.04	0.89
1:A:329:ARG:C	9:A:503:HOH:O	2.29	0.69
1:C:29:ILE:HD11	2:D:102:LEU:HD23	1.79	0.64
1:E:29:ILE:HD11	2:F:102:LEU:HD23	1.87	0.56
1:A:29:ILE:HD11	2:B:102:LEU:HD23	1.88	0.55
1:A:32:ASP:OD1	1:A:33:GLN:N	2.41	0.54
1:C:131:THR:HG21	8:C:510:TAM:H21	1.90	0.53
1:A:53:ASN:C	1:A:53:ASN:HD22	2.13	0.53
1:A:121:ILE:HD13	1:A:257:TYR:CE1	2.46	0.51
1:A:321:ARG:HG3	1:A:321:ARG:HH11	1.76	0.50
1:A:329:ARG:CA	9:A:503:HOH:O	2.60	0.50
1:C:141:ARG:HG3	1:C:141:ARG:HH11	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ASN:HD22	1:A:54:ASN:N	2.09	0.50
1:A:307:LYS:NZ	9:A:501:HOH:O	2.46	0.48
1:A:222:TRP:CZ2	1:A:225:GLY:HA2	2.48	0.47
2:F:150:GLU:OE2	2:F:154:ASN:ND2	2.48	0.47
1:E:222:TRP:CZ2	1:E:225:GLY:HA2	2.50	0.46
1:A:141:ARG:HH11	1:A:141:ARG:HG3	1.80	0.46
1:A:207:ARG:HG2	1:C:221:PRO:HB2	2.00	0.43
1:C:141:ARG:HG3	1:C:141:ARG:NH1	2.34	0.42
1:A:321:ARG:HG3	1:A:321:ARG:NH1	2.33	0.42
1:A:216:ASN:OD1	1:E:212:THR:HG21	2.19	0.42
1:A:325:GLU:O	1:A:327:GLN:NE2	2.45	0.42
1:E:222:TRP:CE2	1:E:225:GLY:HA2	2.55	0.42
1:C:325:GLU:HA	1:C:325:GLU:OE1	2.20	0.41
1:A:222:TRP:CE2	1:A:225:GLY:HA2	2.56	0.41

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	319/323 (99%)	313 (98%)	5 (2%)	1 (0%)	44	50
1	C	315/323 (98%)	309 (98%)	5 (2%)	1 (0%)	44	50
1	E	315/323 (98%)	309 (98%)	5 (2%)	1 (0%)	44	50
2	B	170/174 (98%)	163 (96%)	7 (4%)	0	100	100
2	D	169/174 (97%)	162 (96%)	7 (4%)	0	100	100
2	F	169/174 (97%)	162 (96%)	7 (4%)	0	100	100
All	All	1457/1491 (98%)	1418 (97%)	36 (2%)	3 (0%)	51	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ILE
1	C	62	ILE
1	E	62	ILE

### 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	282/283 (100%)	274 (97%)	8 (3%)	49	58
1	C	278/283 (98%)	270 (97%)	8 (3%)	48	57
1	E	278/283 (98%)	274 (99%)	4 (1%)	71	81
2	B	146/148 (99%)	143 (98%)	3 (2%)	59	68
2	D	145/148 (98%)	141 (97%)	4 (3%)	49	58
2	F	145/148 (98%)	141 (97%)	4 (3%)	49	58
All	All	1274/1293 (98%)	1243 (98%)	31 (2%)	54	64

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	24	THR
1	A	53	ASN
1	A	189	GLN
1	A	190	ASP
1	A	242	VAL
1	A	276	THR
1	A	307	LYS
2	B	39	LYS
2	B	110	LEU
2	B	143	LYS
1	C	18	HIS
1	C	24	THR
1	C	32	ASP
1	C	167	THR
1	C	189	GLN

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Mol	Chain	Res	Type
1	C	208	ARG
1	C	264	LYS
1	C	325	GLU
2	D	60	ASN
2	D	72	GLU
2	D	110	LEU
2	D	143	LYS
1	E	18	HIS
1	E	24	THR
1	E	32	ASP
1	E	189	GLN
2	F	38	LEU
2	F	72	GLU
2	F	110	LEU
2	F	143	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	53	ASN
2	B	53	ASN
2	B	125	GLN
2	D	125	GLN
1	E	22	ASN
1	E	33	GLN
2	F	125	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

36 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	NAG	A	401	1,3	14,14,15	0.49	0	15,19,21	0.92	0
3	NAG	A	402	3,4	14,14,15	0.81	0	15,19,21	1.16	1 (6%)
4	BMA	A	403	3	11,11,12	0.46	0	13,15,17	1.03	1 (7%)
3	NAG	A	404	1	14,14,15	0.75	0	15,19,21	1.60	3 (20%)
3	NAG	A	405	1,3	14,14,15	0.62	1 (7%)	15,19,21	1.56	3 (20%)
3	NAG	A	406	3,4	14,14,15	0.50	0	15,19,21	0.67	0
4	BMA	A	407	3	11,11,12	0.67	0	13,15,17	1.38	2 (15%)
3	NAG	A	408	1,3	14,14,15	0.59	0	15,19,21	1.33	3 (20%)
3	NAG	A	409	3	14,14,15	0.62	0	15,19,21	1.37	1 (6%)
5	SIA	A	410	6	17,20,21	0.51	0	19,28,31	0.64	0
6	GAL	A	411	3,5	11,11,12	0.51	0	13,15,17	0.69	0
3	NAG	A	412	6	15,15,15	0.64	0	21,21,21	1.49	3 (14%)
3	NAG	C	501	1	14,14,15	0.58	0	15,19,21	2.01	2 (13%)
3	NAG	C	502	1	14,14,15	0.70	0	15,19,21	1.93	2 (13%)
3	NAG	C	503	1,3	14,14,15	0.41	0	15,19,21	1.30	3 (20%)
3	NAG	C	504	3,4	14,14,15	0.30	0	15,19,21	1.02	1 (6%)
4	BMA	C	505	3,7	11,11,12	0.23	0	13,15,17	0.98	1 (7%)
7	MAN	C	506	4	11,11,12	0.47	0	13,15,17	0.95	1 (7%)
7	MAN	C	507	4	11,11,12	0.45	0	13,15,17	0.73	0
3	NAG	C	508	1,3	14,14,15	0.38	0	15,19,21	0.90	0
3	NAG	C	509	3	14,14,15	0.59	0	15,19,21	2.20	2 (13%)
8	TAM	C	510	-	7,10,10	0.68	0	9,12,12	0.94	1 (11%)
5	SIA	C	511	6	17,20,21	0.47	0	19,28,31	0.61	0
6	GAL	C	512	3,5	11,11,12	0.58	0	13,15,17	2.16	2 (15%)
3	NAG	C	513	6	15,15,15	0.59	0	21,21,21	1.43	3 (14%)
3	NAG	E	501	1	14,14,15	0.64	0	15,19,21	1.29	1 (6%)
3	NAG	E	502	1,3	14,14,15	0.47	0	15,19,21	1.43	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	E	503	3,4	14,14,15	0.40	0	15,19,21	1.14	2 (13%)
4	BMA	E	504	3,7	11,11,12	0.37	0	13,15,17	1.04	1 (7%)
7	MAN	E	505	4	11,11,12	0.46	0	13,15,17	1.39	1 (7%)
7	MAN	E	506	4	11,11,12	0.50	0	13,15,17	0.98	1 (7%)
3	NAG	E	507	1,3	14,14,15	0.49	0	15,19,21	1.07	1 (6%)
3	NAG	E	508	3	14,14,15	0.55	0	15,19,21	2.26	2 (13%)
8	TAM	E	509	-	7,10,10	0.60	0	9,12,12	1.18	1 (11%)
5	SIA	E	510	6	17,20,21	0.40	0	19,28,31	0.62	0
6	GAL	E	511	5	12,12,12	0.54	0	17,17,17	1.13	1 (5%)

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	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	403	3	-	0/2/19/22	0/1/1/1
3	NAG	A	404	1	-	0/6/23/26	0/1/1/1
3	NAG	A	405	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	406	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	407	3	-	0/2/19/22	0/1/1/1
3	NAG	A	408	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	409	3	-	0/6/23/26	0/1/1/1
5	SIA	A	410	6	-	0/14/34/38	0/1/1/1
6	GAL	A	411	3,5	-	0/2/19/22	0/1/1/1
3	NAG	A	412	6	-	0/6/26/26	0/1/1/1
3	NAG	C	501	1	-	0/6/23/26	0/1/1/1
3	NAG	C	502	1	-	0/6/23/26	0/1/1/1
3	NAG	C	503	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	504	3,4	-	0/6/23/26	0/1/1/1
4	BMA	C	505	3,7	-	0/2/19/22	0/1/1/1
7	MAN	C	506	4	-	0/2/19/22	0/1/1/1
7	MAN	C	507	4	-	0/2/19/22	0/1/1/1
3	NAG	C	508	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	509	3	-	0/6/23/26	0/1/1/1
8	TAM	C	510	-	-	0/12/12/12	0/0/0/0
5	SIA	C	511	6	-	0/14/34/38	0/1/1/1
6	GAL	C	512	3,5	-	0/2/19/22	0/1/1/1
3	NAG	C	513	6	-	0/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	501	1	-	0/6/23/26	0/1/1/1
3	NAG	E	502	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	503	3,4	-	0/6/23/26	0/1/1/1
4	BMA	E	504	3,7	-	0/2/19/22	0/1/1/1
7	MAN	E	505	4	-	0/2/19/22	0/1/1/1
7	MAN	E	506	4	-	0/2/19/22	0/1/1/1
3	NAG	E	507	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	508	3	-	0/6/23/26	0/1/1/1
8	TAM	E	509	-	-	0/12/12/12	0/0/0/0
5	SIA	E	510	6	-	0/14/34/38	0/1/1/1
6	GAL	E	511	5	-	0/2/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	405	NAG	C1-C2	2.06	1.55	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	405	NAG	O5-C1-C2	-3.46	106.67	111.47
3	E	508	NAG	C4-C3-C2	-2.75	106.99	111.02
3	E	502	NAG	O5-C1-C2	-2.67	107.76	111.47
3	A	404	NAG	O5-C1-C2	-2.22	108.39	111.47
3	C	509	NAG	C4-C3-C2	-2.09	107.95	111.02
3	A	408	NAG	C3-C4-C5	-2.09	106.53	110.22
3	A	404	NAG	C4-C3-C2	-2.04	108.03	111.02
3	C	503	NAG	O5-C1-C2	-2.00	108.69	111.47
3	E	503	NAG	C1-C2-N2	2.05	113.99	110.49
4	C	505	BMA	C1-C2-C3	2.06	112.26	109.65
7	C	506	MAN	C1-O5-C5	2.16	115.15	112.17
8	C	510	TAM	C3-C-C2	2.18	114.35	110.50
3	C	503	NAG	C3-C4-C5	2.23	114.14	110.22
4	E	504	BMA	C1-C2-C3	2.24	112.48	109.65
3	A	408	NAG	O4-C4-C5	2.28	115.02	109.28
8	E	509	TAM	C3-C-C1	2.43	114.79	110.50
3	C	503	NAG	C1-O5-C5	2.46	115.56	112.17
3	C	504	NAG	C1-C2-N2	2.46	114.69	110.49
7	E	506	MAN	C1-O5-C5	2.58	115.72	112.17
3	E	507	NAG	C1-C2-N2	2.65	115.02	110.49
6	E	511	GAL	C1-C2-C3	2.69	115.51	110.65
3	A	405	NAG	C1-O5-C5	2.70	115.89	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	407	BMA	C1-O5-C5	2.82	116.05	112.17
3	A	408	NAG	C6-C5-C4	2.85	119.68	113.00
3	C	502	NAG	C3-C4-C5	2.87	115.28	110.22
3	C	513	NAG	C1-C2-C3	2.93	114.54	110.54
3	A	412	NAG	C4-C3-C2	2.99	114.76	110.33
3	E	503	NAG	C1-O5-C5	3.00	116.30	112.17
4	A	403	BMA	C1-O5-C5	3.01	116.31	112.17
3	C	513	NAG	O5-C1-C2	3.10	112.63	109.52
4	A	407	BMA	C1-C2-C3	3.13	113.62	109.65
3	C	501	NAG	C3-C4-C5	3.21	115.86	110.22
3	A	402	NAG	C4-C3-C2	3.24	115.76	111.02
3	C	513	NAG	C4-C3-C2	3.30	115.22	110.33
3	A	412	NAG	O5-C1-C2	3.36	112.89	109.52
3	A	412	NAG	C1-C2-C3	3.49	115.31	110.54
3	E	502	NAG	C1-O5-C5	3.74	117.32	112.17
3	A	405	NAG	C1-C2-N2	3.75	116.89	110.49
7	E	505	MAN	C1-O5-C5	3.89	117.52	112.17
3	A	409	NAG	C4-C3-C2	3.91	116.75	111.02
3	A	404	NAG	C1-O5-C5	3.97	117.63	112.17
3	E	501	NAG	C1-O5-C5	4.41	118.25	112.17
6	C	512	GAL	C1-C2-C3	4.50	115.36	109.65
6	C	512	GAL	C1-O5-C5	5.57	119.85	112.17
3	C	502	NAG	C1-O5-C5	5.63	119.93	112.17
3	C	501	NAG	C1-O5-C5	6.22	120.74	112.17
3	C	509	NAG	C1-O5-C5	7.54	122.56	112.17
3	E	508	NAG	C1-O5-C5	7.96	123.13	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	510	TAM	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	321/323 (99%)	0.05	12 (3%) 42 45	29, 47, 79, 110	0
1	C	317/323 (98%)	-0.19	3 (0%) 84 85	31, 43, 61, 106	0
1	E	317/323 (98%)	-0.09	3 (0%) 84 85	26, 36, 58, 101	0
2	B	172/174 (98%)	0.44	13 (7%) 15 16	26, 55, 90, 119	0
2	D	171/174 (98%)	0.14	7 (4%) 38 41	28, 51, 89, 107	0
2	F	171/174 (98%)	0.37	11 (6%) 20 23	27, 54, 92, 107	0
All	All	1469/1491 (98%)	0.06	49 (3%) 47 51	26, 44, 85, 119	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	PRO	7.0
2	F	171	PHE	5.4
1	C	22	ASN	4.6
2	B	59	THR	4.2
2	B	31	GLY	4.1
1	A	128	THR	4.0
2	B	143	LYS	3.6
2	B	171	PHE	3.5
2	B	147	ALA	3.5
1	C	9	PRO	3.5
2	B	172	GLN	3.3
1	A	160	THR	3.2
1	E	22	ASN	3.2
2	F	143	LYS	3.1
1	A	10	GLY	3.0
2	D	33	GLY	3.0
1	A	127	TRP	3.0
2	B	167	LEU	3.0
2	B	27	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	126	THR	2.9
1	A	159	SER	2.8
1	A	130	VAL	2.8
2	D	167	LEU	2.8
2	B	29	SER	2.8
1	A	208	ARG	2.8
2	B	154	ASN	2.7
2	D	171	PHE	2.7
1	A	143	PRO	2.6
1	E	9	PRO	2.5
2	F	31	GLY	2.5
2	F	168	ASN	2.5
2	F	2	LEU	2.4
2	B	30	GLU	2.4
2	D	161	VAL	2.4
2	F	164	ASP	2.4
1	A	11	ALA	2.3
2	F	167	LEU	2.3
2	D	147	ALA	2.2
1	A	32	ASP	2.2
1	E	81	ASN	2.1
2	F	166	ALA	2.1
2	D	168	ASN	2.1
2	B	146	ASN	2.1
1	C	222	TRP	2.1
2	F	1	GLY	2.0
2	F	147	ALA	2.0
2	D	157	TYR	2.0
2	B	18	ILE	2.0
2	F	30	GLU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 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. 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(Å <sup>2</sup> )	Q<0.9
8	TAM	C	510	11/11	0.59	0.59	17.98	63,75,79,81	0
3	NAG	E	501	14/15	0.83	0.26	16.13	56,67,70,70	0
3	NAG	A	408	14/15	0.95	0.18	4.58	36,42,53,64	0
3	NAG	E	507	14/15	0.94	0.12	2.07	36,46,53,66	0
3	NAG	A	406	14/15	0.88	0.26	1.80	77,81,86,86	0
5	SIA	A	410	20/21	0.90	0.17	1.05	54,64,67,68	0
3	NAG	E	503	14/15	0.89	0.14	0.93	51,61,71,73	0
5	SIA	E	510	20/21	0.97	0.10	-0.62	32,38,41,42	0
3	NAG	C	504	14/15	0.95	0.12	-0.70	40,46,58,58	0
5	SIA	C	511	20/21	0.96	0.10	-0.76	41,44,48,49	0
3	NAG	C	508	14/15	0.94	0.10	-1.14	39,46,52,62	0
3	NAG	C	503	14/15	0.94	0.10	-2.08	36,41,48,49	0
4	BMA	A	407	11/12	0.81	0.22	-	85,88,91,91	0
7	MAN	C	507	11/12	0.69	0.40	-	91,94,96,98	0
3	NAG	E	502	14/15	0.95	0.15	-	47,53,59,61	0
6	GAL	C	512	11/12	0.88	0.16	-	60,74,82,83	0
8	TAM	E	509	11/11	0.73	0.20	-	68,79,80,81	0
6	GAL	A	411	11/12	0.82	0.23	-	81,88,96,98	0
3	NAG	A	404	14/15	0.83	0.18	-	51,62,66,68	0
3	NAG	A	402	14/15	0.79	0.38	-	88,94,104,111	0
3	NAG	A	405	14/15	0.91	0.19	-	65,70,78,80	0
4	BMA	E	504	11/12	0.84	0.17	-	81,88,95,101	0
7	MAN	C	506	11/12	0.76	0.26	-	99,103,108,109	0
3	NAG	C	501	14/15	0.75	0.25	-	63,75,81,82	0
7	MAN	E	506	11/12	0.76	0.34	-	99,106,109,110	0
3	NAG	C	513	15/15	0.73	0.32	-	93,100,107,109	0
3	NAG	A	401	14/15	0.94	0.21	-	54,62,71,76	0
4	BMA	C	505	11/12	0.90	0.15	-	65,73,84,88	0
3	NAG	C	502	14/15	0.68	0.38	-	68,80,83,87	0
6	GAL	E	511	12/12	0.89	0.22	-	46,68,72,76	0
3	NAG	C	509	14/15	0.80	0.27	-	71,77,85,89	0
3	NAG	E	508	14/15	0.76	0.25	-	71,86,92,96	0
7	MAN	E	505	11/12	0.69	0.42	-	100,102,105,107	0
3	NAG	A	409	14/15	0.72	0.31	-	75,81,91,92	0
3	NAG	A	412	15/15	0.78	0.35	-	104,109,111,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	BMA	A	403	11/12	0.65	0.32	-	101,107,112,113	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.