



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:01 am GMT

PDB ID : 4WSW  
Title : The crystal structure of hemagglutinin from A/green-winged teal/Texas/Y171/2006 influenza virus  
Authors : Yang, H.; Carney, P.J.; Chang, J.C.; Villanueva, J.M.; Stevens, J.  
Deposited on : 2014-10-28  
Resolution : 2.80 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 : 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

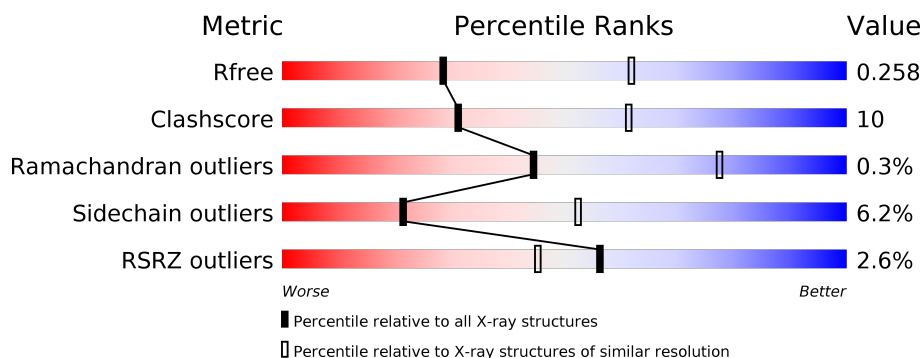
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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>78%</div> <div>17%</div> <div>••</div> </div>
1	C	327	<div> <div>3%</div> <div>77%</div> <div>17%</div> <div>••</div> </div>
1	E	327	<div> <div>2%</div> <div>76%</div> <div>18%</div> <div>••</div> </div>
2	B	182	<div> <div>4%</div> <div>79%</div> <div>14%</div> <div>•• 5%</div> </div>
2	D	182	<div> <div>3%</div> <div>77%</div> <div>16%</div> <div>• 5%</div> </div>
2	F	182	<div> <div>4%</div> <div>68%</div> <div>23%</div> <div>•• 5%</div> </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
3	NAG	A	501	X	-	-	-
3	NAG	B	301	X	-	-	-
3	NAG	D	201	X	-	-	-
3	NAG	E	402	-	-	-	X
3	NAG	F	301	X	-	-	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11634 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

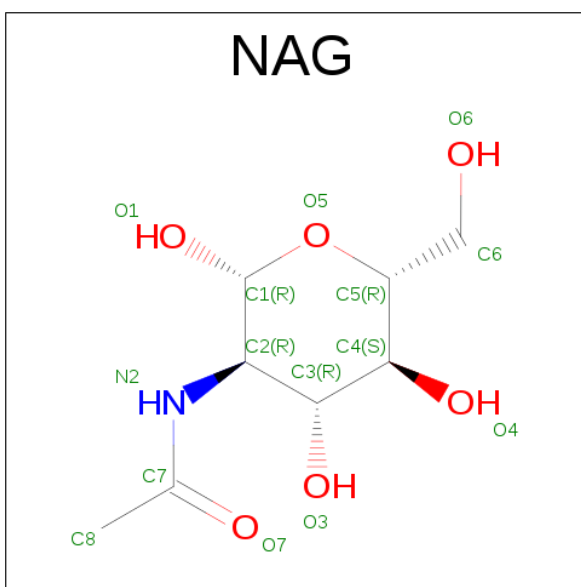
- Molecule 1 is a protein called Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2427	1504	432	476	15			
1	C	319	Total	C	N	O	S	0	0	0
			2427	1504	432	476	15			
1	E	319	Total	C	N	O	S	0	0	0
			2427	1504	432	476	15			

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1395	863	242	282	8			
2	D	172	Total	C	N	O	S	0	0	0
			1395	863	242	282	8			
2	F	172	Total	C	N	O	S	0	0	0
			1395	863	242	282	8			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

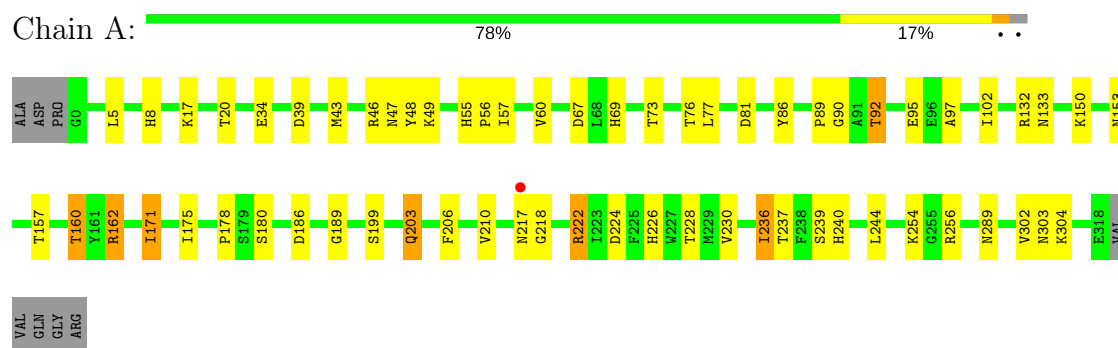


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1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

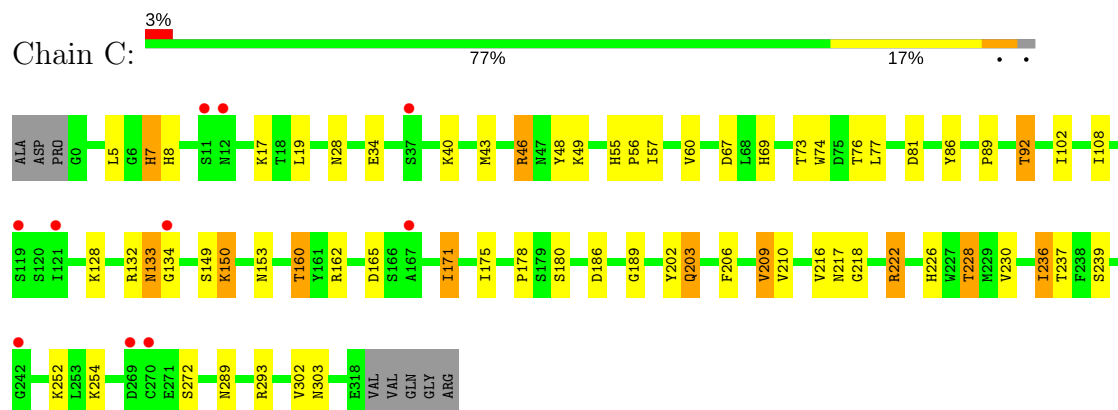
### 3 Residue-property plots [i](#)

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.

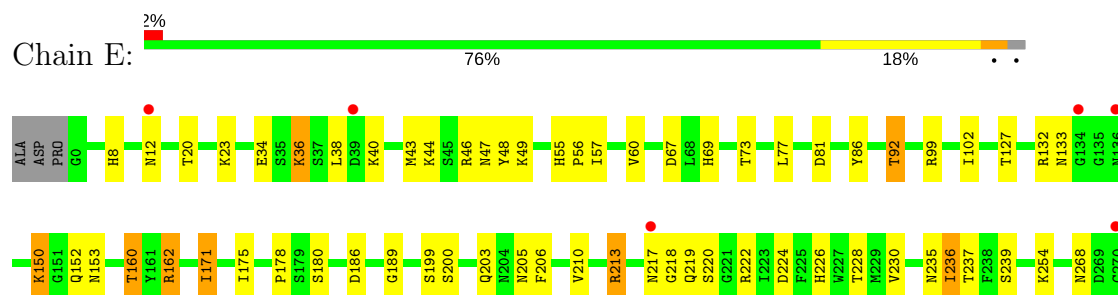
#### • Molecule 1: Hemagglutinin HA1 chain



#### • Molecule 1: Hemagglutinin HA1 chain

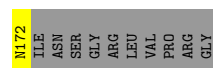
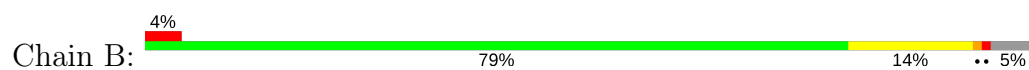


#### • Molecule 1: Hemagglutinin HA1 chain

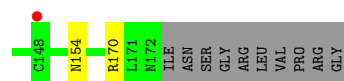
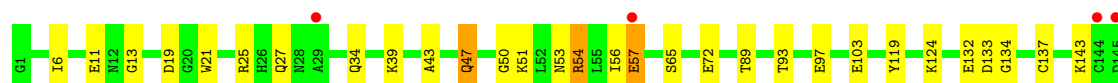
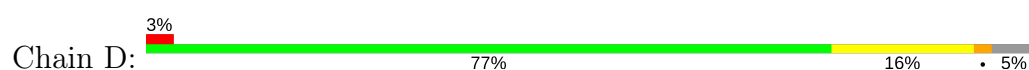




• Molecule 2: Hemagglutinin HA2 chain



• Molecule 2: Hemagglutinin HA2 chain



• Molecule 2: Hemagglutinin HA2 chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.92Å 144.63Å 209.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 49.28 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (50.00-2.80) 98.7 (49.28-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.09 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.224 , 0.258 0.225 , 0.258	Depositor DCC
$R_{free}$ test set	1975 reflections (3.79%)	DCC
Wilson B-factor (Å <sup>2</sup> )	68.1	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.1	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	0.93	EDS
Total number of atoms	11634	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.64	0/2475	0.79	0/3349
1	C	0.63	0/2475	0.83	2/3349 (0.1%)
1	E	0.61	0/2475	0.80	1/3349 (0.0%)
2	B	0.59	0/1420	0.73	1/1915 (0.1%)
2	D	0.56	0/1420	0.73	0/1915
2	F	0.66	0/1420	0.87	5/1915 (0.3%)
All	All	0.62	0/11685	0.80	9/15792 (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	F	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	127	ARG	NE-CZ-NH1	6.32	123.46	120.30
2	F	121	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	E	12	ASN	N-CA-CB	-5.77	100.21	110.60
2	F	129	ASN	N-CA-CB	-5.63	100.46	110.60
2	B	171	LEU	CA-CB-CG	5.52	128.00	115.30
1	C	222	ARG	NE-CZ-NH1	5.25	122.93	120.30
2	F	161	GLN	N-CA-CB	-5.16	101.32	110.60
1	C	46	ARG	NE-CZ-NH1	5.13	122.87	120.30
2	F	74	GLU	N-CA-CB	-5.03	101.55	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	73	ILE	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	2427	0	2375	52	0
1	C	2427	0	2376	58	0
1	E	2427	0	2376	59	0
2	B	1395	0	1298	26	0
2	D	1395	0	1299	31	0
2	F	1395	0	1299	50	0
3	A	42	0	39	1	0
3	B	28	0	26	2	0
3	C	42	0	39	6	0
3	D	14	0	13	1	0
3	E	28	0	26	0	0
3	F	14	0	13	1	0
All	All	11634	0	11179	235	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 10.

All (235) 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:162:ARG:NH1	1:E:235:ASN:OD1	1.84	1.10
1:C:209:VAL:HG21	1:E:205:ASN:CB	1.83	1.07
2:F:128:GLN:OE1	2:F:170:ARG:NH1	1.89	1.05
2:B:171:LEU:O	2:B:171:LEU:HD23	1.62	0.99
1:A:8:HIS:HD2	2:B:21:TRP:HA	1.23	0.99
2:D:170:ARG:NH1	2:F:128:GLN:HE21	1.65	0.95
1:C:132:ARG:O	1:C:133:ASN:HB2	1.66	0.94
1:A:8:HIS:CD2	2:B:21:TRP:HA	2.04	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:HIS:HD2	2:F:21:TRP:HA	1.35	0.90
1:C:209:VAL:HG21	1:E:205:ASN:HB2	1.53	0.90
1:C:8:HIS:HD2	2:D:21:TRP:HA	1.35	0.89
1:A:217:ASN:N	1:A:218:GLY:HA3	1.88	0.88
1:A:203:GLN:NE2	1:E:224:ASP:OD1	2.09	0.85
1:E:217:ASN:N	1:E:218:GLY:HA3	1.91	0.85
1:E:8:HIS:CD2	2:F:21:TRP:HA	2.14	0.82
2:B:89:THR:O	2:B:93:THR:HG23	1.80	0.81
2:F:89:THR:O	2:F:93:THR:HG23	1.80	0.81
1:C:8:HIS:CD2	2:D:21:TRP:HA	2.15	0.81
2:D:89:THR:O	2:D:93:THR:HG23	1.81	0.80
1:E:23:LYS:O	1:E:23:LYS:HG2	1.83	0.77
2:B:47:GLN:HE22	2:B:110:MET:CE	1.97	0.77
1:C:209:VAL:HG21	1:E:205:ASN:HB3	1.67	0.76
1:E:34:GLU:OE2	1:E:36:LYS:HG2	1.85	0.75
1:E:171:ILE:HD11	1:E:236:ILE:HD12	1.68	0.74
2:F:125:GLN:NE2	2:F:155:ASN:HA	2.01	0.73
1:A:157:THR:HB	1:A:240:HIS:CE1	2.24	0.73
1:A:86:TYR:OH	1:A:92:THR:HG23	1.90	0.71
1:E:217:ASN:H	1:E:218:GLY:HA3	1.54	0.71
1:A:217:ASN:H	1:A:218:GLY:HA3	1.53	0.70
2:F:164:GLU:OE1	2:F:165:GLU:N	2.24	0.70
1:E:86:TYR:OH	1:E:92:THR:HG23	1.93	0.69
1:C:86:TYR:OH	1:C:92:THR:HG23	1.92	0.69
3:C:501:NAG:H4	3:C:502:NAG:H82	1.74	0.68
1:C:217:ASN:H	1:C:218:GLY:HA3	1.58	0.68
1:A:5:LEU:HD22	2:B:119:TYR:HA	1.75	0.68
2:D:133:ASP:OD2	2:D:137:CYS:HB2	1.93	0.68
1:C:217:ASN:N	1:C:218:GLY:HA3	2.08	0.67
2:F:164:GLU:N	2:F:164:GLU:OE1	2.28	0.67
2:B:171:LEU:CD2	2:B:171:LEU:O	2.42	0.66
2:F:171:LEU:O	2:F:172:ASN:ND2	2.30	0.65
2:F:165:GLU:C	2:F:165:GLU:OE1	2.34	0.65
1:E:303:ASN:H	2:F:93:THR:CG2	2.10	0.65
2:D:53:ASN:O	2:D:57:GLU:OE2	2.15	0.64
1:A:224:ASP:OD1	1:C:203:GLN:NE2	2.32	0.63
3:C:503:NAG:O7	3:C:503:NAG:O3	2.16	0.63
2:F:25:ARG:NH2	2:F:34:GLN:NE2	2.47	0.62
1:A:97:ALA:HB2	2:F:76:GLN:OE1	2.00	0.61
1:E:302:VAL:HA	2:F:93:THR:HG22	1.80	0.61
1:E:171:ILE:HD11	1:E:230:VAL:CG2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:LEU:O	2:B:172:ASN:ND2	2.32	0.61
1:A:5:LEU:CD2	2:B:119:TYR:HA	2.30	0.61
1:E:38:LEU:HD22	1:E:40:LYS:HB2	1.82	0.60
2:F:129:ASN:ND2	2:F:157:TYR:OH	2.35	0.60
3:F:301:NAG:O7	3:F:301:NAG:O3	2.17	0.60
1:C:28:ASN:OD1	3:C:501:NAG:H61	2.00	0.60
1:C:209:VAL:CG2	1:E:205:ASN:HB2	2.29	0.60
2:F:129:ASN:HD21	2:F:162:TYR:HB2	1.67	0.60
1:A:43:MET:HE2	1:A:48:TYR:HB3	1.82	0.60
2:F:25:ARG:NH2	2:F:34:GLN:HE21	2.00	0.60
1:A:17:LYS:HE3	2:D:54:ARG:HH21	1.66	0.59
1:E:49:LYS:HE3	1:E:69:HIS:ND1	2.17	0.59
1:A:49:LYS:HE3	1:A:69:HIS:ND1	2.17	0.59
2:D:25:ARG:NH2	2:D:34:GLN:OE1	2.31	0.59
2:F:158:ASP:OD2	2:F:160:THR:OG1	2.21	0.58
1:C:49:LYS:HE3	1:C:69:HIS:ND1	2.18	0.58
2:B:25:ARG:NH2	2:B:34:GLN:OE1	2.31	0.58
2:D:133:ASP:OD1	2:D:134:GLY:N	2.37	0.57
1:E:171:ILE:CD1	1:E:236:ILE:HD12	2.34	0.57
1:E:43:MET:HE1	1:E:46:ARG:HD3	1.87	0.57
1:C:217:ASN:OD1	1:C:218:GLY:HA3	2.05	0.57
1:E:303:ASN:H	2:F:93:THR:HG21	1.69	0.57
1:A:302:VAL:HA	2:B:93:THR:HG22	1.88	0.56
1:C:28:ASN:OD1	3:C:501:NAG:C6	2.54	0.56
1:C:43:MET:HE1	1:C:46:ARG:HD3	1.88	0.56
2:B:50:GLY:HA3	1:E:20:THR:O	2.06	0.55
2:F:162:TYR:C	2:F:164:GLU:OE1	2.44	0.55
2:F:162:TYR:O	2:F:164:GLU:OE1	2.24	0.55
1:A:240:HIS:HD2	1:A:244:LEU:HD22	1.71	0.55
1:A:171:ILE:HD11	1:A:230:VAL:HG21	1.89	0.55
1:C:165:ASP:OD2	1:C:252:LYS:NZ	2.41	0.54
1:A:92:THR:O	1:A:95:GLU:HG2	2.08	0.54
1:E:43:MET:HE2	1:E:48:TYR:HB3	1.90	0.54
2:F:165:GLU:OE2	2:F:169:ASN:ND2	2.41	0.54
1:C:171:ILE:HD11	1:C:230:VAL:HG21	1.90	0.54
1:A:217:ASN:N	1:A:218:GLY:CA	2.67	0.53
1:A:162:ARG:NH2	3:A:503:NAG:H4	2.24	0.53
1:C:74:TRP:CH2	1:C:108:ILE:HD12	2.44	0.53
1:E:81:ASP:O	1:E:81:ASP:OD1	2.26	0.53
1:E:217:ASN:N	1:E:218:GLY:CA	2.69	0.53
1:E:127:THR:OG1	1:E:219:GLN:NE2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:HIS:CD2	1:A:244:LEU:CD2	2.91	0.53
1:C:43:MET:HE2	1:C:48:TYR:HB3	1.91	0.53
1:C:202:TYR:CD1	1:C:228:THR:HG21	2.44	0.53
2:F:53:ASN:O	2:F:57:GLU:OE2	2.27	0.53
1:A:43:MET:CE	1:A:48:TYR:HB3	2.39	0.53
3:D:201:NAG:O3	3:D:201:NAG:O7	2.25	0.52
1:E:153:ASN:HA	1:E:189:GLY:HA2	1.91	0.52
1:A:81:ASP:HB3	2:B:70:PHE:CE1	2.45	0.52
1:A:81:ASP:HB3	2:B:70:PHE:CD1	2.44	0.52
2:B:74:GLU:OE2	2:B:76:GLN:HB3	2.09	0.52
1:E:178:PRO:HG2	1:E:210:VAL:HG22	1.92	0.52
1:A:178:PRO:HG2	1:A:210:VAL:HG22	1.92	0.52
2:F:76:GLN:HG2	2:F:77:ILE:HD12	1.91	0.52
2:D:170:ARG:HH12	2:F:128:GLN:HE21	1.54	0.51
2:B:134:GLY:HA2	2:D:124:LYS:HD3	1.92	0.51
2:D:170:ARG:NH1	2:F:128:GLN:NE2	2.46	0.51
1:E:171:ILE:HD11	1:E:230:VAL:HG22	1.93	0.51
1:C:5:LEU:HD22	2:D:119:TYR:HA	1.93	0.51
2:F:25:ARG:HH21	2:F:34:GLN:NE2	2.08	0.51
1:A:240:HIS:CD2	1:A:244:LEU:HD23	2.46	0.50
2:B:47:GLN:NE2	2:B:110:MET:SD	2.84	0.50
1:C:7:HIS:HD1	2:D:13:GLY:HA2	1.76	0.50
1:E:67:ASP:OD1	1:E:132:ARG:NH1	2.44	0.50
1:C:7:HIS:CE1	2:D:13:GLY:HA2	2.46	0.50
1:A:153:ASN:HA	1:A:189:GLY:HA2	1.94	0.50
2:B:47:GLN:HE22	2:B:110:MET:HE1	1.75	0.50
1:C:178:PRO:HG2	1:C:210:VAL:HG22	1.94	0.50
1:C:7:HIS:ND1	2:D:13:GLY:HA2	2.27	0.50
2:D:53:ASN:O	2:D:57:GLU:CD	2.50	0.50
1:C:55:HIS:CD2	1:C:56:PRO:HD2	2.47	0.50
1:A:67:ASP:OD1	1:A:132:ARG:NH1	2.44	0.50
1:A:256:ARG:NH2	2:B:64:GLU:OE2	2.44	0.50
1:A:240:HIS:HD2	1:A:244:LEU:CD2	2.25	0.49
1:A:303:ASN:H	2:B:93:THR:CG2	2.24	0.49
1:C:43:MET:CE	1:C:48:TYR:HB3	2.42	0.49
1:E:43:MET:CE	1:E:48:TYR:HB3	2.42	0.49
2:F:165:GLU:OE1	2:F:166:ALA:N	2.45	0.49
2:B:75:HIS:CE1	3:B:301:NAG:H62	2.47	0.49
2:F:129:ASN:ND2	2:F:162:TYR:HB2	2.27	0.49
1:A:160:THR:HG22	1:A:237:THR:HG23	1.94	0.49
1:C:302:VAL:HA	2:D:93:THR:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:THR:HG22	1:E:237:THR:HG23	1.94	0.49
2:D:56:ILE:C	2:D:57:GLU:CD	2.71	0.49
1:C:217:ASN:OD1	1:C:218:GLY:CA	2.61	0.49
1:C:81:ASP:O	1:C:81:ASP:OD1	2.31	0.49
1:A:43:MET:HE1	1:A:46:ARG:HD3	1.94	0.48
1:C:165:ASP:OD2	1:C:252:LYS:CE	2.61	0.48
1:E:152:GLN:HG2	1:E:153:ASN:O	2.14	0.48
3:B:301:NAG:O7	3:B:301:NAG:O3	2.30	0.48
3:C:501:NAG:H4	3:C:502:NAG:C8	2.43	0.48
1:A:89:PRO:O	1:A:222:ARG:HG3	2.14	0.48
1:E:55:HIS:CD2	1:E:56:PRO:HD2	2.49	0.48
2:F:25:ARG:HH21	2:F:34:GLN:HE21	1.62	0.48
2:D:56:ILE:O	2:D:57:GLU:OE2	2.32	0.48
1:C:153:ASN:HA	1:C:189:GLY:HA2	1.96	0.48
1:E:44:LYS:HG2	1:E:268:ASN:O	2.13	0.48
1:C:175:ILE:HD12	1:C:226:HIS:CD2	2.49	0.47
1:C:222:ARG:HH21	1:E:200:SER:HA	1.79	0.47
2:B:47:GLN:NE2	2:B:110:MET:CE	2.70	0.47
1:C:67:ASP:OD1	1:C:132:ARG:NH1	2.47	0.47
1:C:160:THR:HG22	1:C:237:THR:HG23	1.96	0.47
2:F:125:GLN:HE22	2:F:155:ASN:HA	1.78	0.47
2:D:53:ASN:C	2:D:57:GLU:OE2	2.52	0.47
1:C:217:ASN:N	1:C:218:GLY:CA	2.78	0.47
2:D:51:LYS:NZ	2:D:103:GLU:OE1	2.43	0.47
1:E:284:LYS:HB3	2:F:56:ILE:HG23	1.97	0.47
2:B:124:LYS:HD3	2:F:134:GLY:HA2	1.97	0.46
1:E:213:ARG:HD2	1:E:222:ARG:HG2	1.97	0.46
1:E:199:SER:HB3	1:E:236:ILE:HD13	1.97	0.46
1:A:175:ILE:HD11	1:A:206:PHE:CG	2.50	0.46
1:A:55:HIS:HD2	1:A:57:ILE:H	1.62	0.46
1:A:240:HIS:CD2	1:A:244:LEU:HD22	2.51	0.46
2:F:164:GLU:CD	2:F:165:GLU:N	2.69	0.46
1:E:153:ASN:HA	1:E:189:GLY:CA	2.45	0.46
1:E:150:LYS:O	1:E:186:ASP:O	2.33	0.45
1:E:38:LEU:CD2	1:E:40:LYS:HB2	2.46	0.45
1:C:175:ILE:HD11	1:C:206:PHE:CG	2.51	0.45
1:C:7:HIS:HD2	2:D:6:ILE:HG12	1.81	0.45
1:C:133:ASN:HA	1:C:134:GLY:C	2.36	0.45
1:C:209:VAL:HG21	1:E:205:ASN:CG	2.36	0.45
1:A:20:THR:O	2:D:50:GLY:HA3	2.16	0.45
1:A:43:MET:HE2	1:A:48:TYR:CB	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:HIS:CD2	2:D:6:ILE:HG12	2.52	0.45
2:F:35:ALA:HB3	2:F:153:ARG:HH11	1.82	0.45
1:C:303:ASN:H	2:D:93:THR:CG2	2.30	0.45
1:E:175:ILE:HD11	1:E:206:PHE:CG	2.52	0.44
2:F:51:LYS:NZ	2:F:103:GLU:OE1	2.43	0.44
2:F:74:GLU:CD	2:F:74:GLU:C	2.76	0.44
2:F:75:HIS:CE1	2:F:79:ASN:ND2	2.86	0.44
1:A:153:ASN:HA	1:A:189:GLY:CA	2.47	0.44
2:D:43:ALA:O	2:D:47:GLN:HG3	2.17	0.44
1:A:73:THR:HG22	1:A:254:LYS:NZ	2.33	0.44
1:C:5:LEU:CD2	2:D:119:TYR:HA	2.48	0.44
1:C:153:ASN:HA	1:C:189:GLY:CA	2.47	0.43
1:C:46:ARG:NH1	1:C:272:SER:O	2.51	0.43
1:A:55:HIS:CD2	1:A:56:PRO:HD2	2.53	0.43
1:C:150:LYS:O	1:C:186:ASP:O	2.36	0.43
2:F:35:ALA:CB	2:F:153:ARG:HH11	2.31	0.43
1:C:230:VAL:HG22	1:C:236:ILE:CD1	2.48	0.43
1:C:73:THR:HG22	1:C:254:LYS:NZ	2.33	0.43
1:E:55:HIS:HD2	1:E:57:ILE:H	1.66	0.43
2:D:143:LYS:HD3	2:D:143:LYS:N	2.33	0.43
1:E:305:LYS:HD2	1:E:305:LYS:N	2.33	0.43
2:F:164:GLU:HG2	2:F:165:GLU:HB2	2.01	0.43
1:A:175:ILE:HD12	1:A:226:HIS:CD2	2.54	0.43
1:A:150:LYS:O	1:A:186:ASP:O	2.37	0.43
1:C:55:HIS:HD2	1:C:57:ILE:H	1.67	0.43
1:E:302:VAL:CA	2:F:93:THR:HG22	2.46	0.43
1:A:230:VAL:HG22	1:A:236:ILE:CD1	2.49	0.42
1:E:133:ASN:OD1	1:E:133:ASN:N	2.52	0.42
1:C:60:VAL:HG21	1:C:102:ILE:HD11	2.02	0.42
1:E:34:GLU:O	1:E:289:ASN:HB2	2.20	0.42
1:C:89:PRO:HG3	1:C:216:VAL:O	2.20	0.42
2:D:56:ILE:HB	2:D:57:GLU:OE1	2.19	0.42
1:E:73:THR:HG22	1:E:254:LYS:NZ	2.34	0.42
2:B:123:ARG:NH2	2:F:132:GLU:OE1	2.49	0.42
2:B:171:LEU:CG	2:B:171:LEU:O	2.68	0.42
1:E:199:SER:HB3	1:E:236:ILE:CD1	2.50	0.42
1:A:90:GLY:HA2	1:A:222:ARG:HG2	2.02	0.42
1:A:217:ASN:OD1	1:A:217:ASN:N	2.53	0.41
1:A:43:MET:CE	1:A:76:THR:HG21	2.50	0.41
1:C:34:GLU:O	1:C:289:ASN:HB2	2.20	0.41
1:E:175:ILE:HD12	1:E:226:HIS:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:230:VAL:HG22	1:E:236:ILE:CD1	2.50	0.41
1:C:132:ARG:O	1:C:133:ASN:CB	2.48	0.41
1:C:7:HIS:CE1	2:D:13:GLY:CA	3.03	0.41
1:E:284:LYS:HA	1:E:284:LYS:HD3	1.75	0.41
2:B:56:ILE:O	2:B:57:GLU:HG2	2.21	0.41
1:E:303:ASN:H	2:F:93:THR:HG22	1.84	0.41
1:C:43:MET:CE	1:C:76:THR:HG21	2.50	0.41
2:F:118:LEU:HA	2:F:121:ARG:HH11	1.85	0.41
2:F:56:ILE:O	2:F:57:GLU:HG2	2.21	0.41
1:E:60:VAL:HG21	1:E:102:ILE:HD11	2.03	0.41
2:F:126:LEU:O	2:F:129:ASN:HB3	2.21	0.41
1:A:34:GLU:O	1:A:289:ASN:HB2	2.20	0.40
3:C:503:NAG:C7	3:C:503:NAG:HO3	2.26	0.40
1:E:171:ILE:CD1	1:E:230:VAL:CG2	2.97	0.40
2:F:164:GLU:CG	2:F:165:GLU:N	2.84	0.40
1:C:19:LEU:O	2:F:54:ARG:NH1	2.54	0.40
2:F:75:HIS:CE1	2:F:79:ASN:HD21	2.38	0.40
1:A:199:SER:HB3	1:A:236:ILE:HD13	2.03	0.40
1:A:289:ASN:OD1	1:A:304:LYS:O	2.39	0.40
1:A:60:VAL:HG21	1:A:102:ILE:HD11	2.03	0.40
2:F:143:LYS:C	2:F:143:LYS:HD2	2.42	0.40
1:E:289:ASN:OD1	1:E:304:LYS:O	2.39	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	317/327 (97%)	298 (94%)	18 (6%)	1 (0%)	44	77
1	C	317/327 (97%)	300 (95%)	16 (5%)	1 (0%)	44	77
1	E	317/327 (97%)	298 (94%)	19 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	170/182 (93%)	165 (97%)	5 (3%)	0	100	100
2	D	170/182 (93%)	162 (95%)	7 (4%)	1 (1%)	28	62
2	F	170/182 (93%)	164 (96%)	4 (2%)	2 (1%)	15	44
All	All	1461/1527 (96%)	1387 (95%)	69 (5%)	5 (0%)	44	77

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	133	ASN
2	F	74	GLU
2	D	72	GLU
2	F	164	GLU
1	A	39	ASP

### 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	272/278 (98%)	259 (95%)	13 (5%)	30	63
1	C	272/278 (98%)	254 (93%)	18 (7%)	19	49
1	E	272/278 (98%)	255 (94%)	17 (6%)	21	51
2	B	147/155 (95%)	138 (94%)	9 (6%)	22	53
2	D	147/155 (95%)	136 (92%)	11 (8%)	16	41
2	F	147/155 (95%)	137 (93%)	10 (7%)	18	47
All	All	1257/1299 (97%)	1179 (94%)	78 (6%)	21	52

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	77	LEU
1	A	92	THR

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Mol	Chain	Res	Type
1	A	133	ASN
1	A	160	THR
1	A	162	ARG
1	A	171	ILE
1	A	180	SER
1	A	203	GLN
1	A	222	ARG
1	A	228	THR
1	A	236	ILE
1	A	239	SER
2	B	19	ASP
2	B	27	GLN
2	B	54	ARG
2	B	67	GLU
2	B	72	GLU
2	B	76	GLN
2	B	87	SER
2	B	132	GLU
2	B	171	LEU
1	C	7	HIS
1	C	17	LYS
1	C	40	LYS
1	C	77	LEU
1	C	92	THR
1	C	128	LYS
1	C	149	SER
1	C	150	LYS
1	C	160	THR
1	C	162	ARG
1	C	171	ILE
1	C	180	SER
1	C	203	GLN
1	C	209	VAL
1	C	228	THR
1	C	236	ILE
1	C	239	SER
1	C	293	ARG
2	D	11	GLU
2	D	19	ASP
2	D	27	GLN
2	D	39	LYS
2	D	47	GLN

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Mol	Chain	Res	Type
2	D	54	ARG
2	D	57	GLU
2	D	65	SER
2	D	97	GLU
2	D	132	GLU
2	D	154	ASN
1	E	36	LYS
1	E	47	ASN
1	E	77	LEU
1	E	92	THR
1	E	99	ARG
1	E	150	LYS
1	E	160	THR
1	E	162	ARG
1	E	171	ILE
1	E	180	SER
1	E	203	GLN
1	E	213	ARG
1	E	220	SER
1	E	228	THR
1	E	236	ILE
1	E	239	SER
1	E	305	LYS
2	F	19	ASP
2	F	27	GLN
2	F	54	ARG
2	F	87	SER
2	F	110	MET
2	F	114	GLU
2	F	132	GLU
2	F	139	GLU
2	F	143	LYS
2	F	164	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	HIS
1	A	8	HIS
1	A	21	ASN
1	A	55	HIS
1	A	133	ASN

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Mol	Chain	Res	Type
1	A	226	HIS
1	A	240	HIS
1	A	289	ASN
2	B	47	GLN
1	C	8	HIS
1	C	55	HIS
1	C	133	ASN
1	C	226	HIS
1	C	289	ASN
2	D	47	GLN
2	D	147	ASN
1	E	7	HIS
1	E	8	HIS
1	E	21	ASN
1	E	55	HIS
1	E	203	GLN
1	E	226	HIS
1	E	240	HIS
2	F	30	GLN
2	F	34	GLN
2	F	79	ASN
2	F	125	GLN
2	F	129	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	$\# Z  > 2$
3	NAG	A	501	1	14,14,15	0.29	0	15,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	502	1	14,14,15	0.96	1 (7%)	15,19,21	1.90	7 (46%)
3	NAG	A	503	1	14,14,15	0.29	0	15,19,21	0.57	0
3	NAG	B	301	2	14,14,15	0.29	0	15,19,21	0.57	0
3	NAG	B	302	2	14,14,15	0.84	1 (7%)	15,19,21	2.03	2 (13%)
3	NAG	C	501	1	14,14,15	1.04	1 (7%)	15,19,21	1.31	1 (6%)
3	NAG	C	502	1	14,14,15	0.63	0	15,19,21	3.05	4 (26%)
3	NAG	C	503	1	14,14,15	0.29	0	15,19,21	0.57	0
3	NAG	D	201	2	14,14,15	0.86	1 (7%)	15,19,21	1.62	5 (33%)
3	NAG	E	401	1	14,14,15	0.28	0	15,19,21	0.58	0
3	NAG	E	402	1	14,14,15	0.49	0	15,19,21	1.52	1 (6%)
3	NAG	F	301	2	14,14,15	0.28	0	15,19,21	0.57	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
3	NAG	A	501	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	502	1	-	0/6/23/26	0/1/1/1
3	NAG	A	503	1	-	0/6/23/26	0/1/1/1
3	NAG	B	301	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	B	302	2	-	0/6/23/26	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	-	0/6/23/26	0/1/1/1
3	NAG	D	201	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	E	401	1	-	0/6/23/26	0/1/1/1
3	NAG	E	402	1	-	0/6/23/26	0/1/1/1
3	NAG	F	301	2	1/1/5/7	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	NAG	C1-C2	2.44	1.55	1.52
3	D	201	NAG	C1-C2	2.74	1.56	1.52
3	A	502	NAG	C1-C2	2.76	1.56	1.52
3	C	501	NAG	C1-C2	3.21	1.56	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	NAG	C4-C3-C2	-4.21	104.85	111.02
3	B	302	NAG	C3-C4-C5	-3.21	104.56	110.22
3	A	502	NAG	O5-C1-C2	-3.20	107.02	111.47
3	D	201	NAG	O5-C1-C2	-2.61	107.84	111.47
3	D	201	NAG	O7-C7-C8	-2.55	117.42	122.06
3	C	502	NAG	O7-C7-C8	-2.53	117.45	122.06
3	A	502	NAG	O3-C3-C4	-2.51	104.90	110.36
3	A	502	NAG	C6-C5-C4	-2.34	107.53	113.00
3	C	501	NAG	O7-C7-C8	-2.16	118.13	122.06
3	A	502	NAG	O7-C7-C8	-2.13	118.18	122.06
3	A	502	NAG	C1-C2-N2	2.01	113.92	110.49
3	D	201	NAG	C2-N2-C7	2.10	126.00	122.94
3	D	201	NAG	O3-C3-C2	2.13	113.94	109.39
3	A	502	NAG	C4-C3-C2	2.35	114.47	111.02
3	D	201	NAG	C1-O5-C5	2.81	116.04	112.17
3	A	502	NAG	C1-O5-C5	3.15	116.51	112.17
3	E	402	NAG	C1-O5-C5	4.57	118.46	112.17
3	C	502	NAG	C1-C2-N2	4.84	118.76	110.49
3	B	302	NAG	C1-O5-C5	5.99	120.42	112.17
3	C	502	NAG	C1-O5-C5	9.09	124.69	112.17

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	F	301	NAG	C1
3	B	301	NAG	C1
3	A	501	NAG	C1
3	D	201	NAG	C1

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	NAG	1	0
3	B	301	NAG	2	0
3	C	501	NAG	4	0
3	C	502	NAG	2	0
3	C	503	NAG	2	0
3	D	201	NAG	1	0
3	F	301	NAG	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

12 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	501	1	14,14,15	0.29	0	15,19,21	0.56	0
3	NAG	A	502	1	14,14,15	0.96	1 (7%)	15,19,21	1.90	7 (46%)
3	NAG	A	503	1	14,14,15	0.29	0	15,19,21	0.57	0
3	NAG	B	301	2	14,14,15	0.29	0	15,19,21	0.57	0
3	NAG	B	302	2	14,14,15	0.84	1 (7%)	15,19,21	2.03	2 (13%)
3	NAG	C	501	1	14,14,15	1.04	1 (7%)	15,19,21	1.31	1 (6%)
3	NAG	C	502	1	14,14,15	0.63	0	15,19,21	3.05	4 (26%)
3	NAG	C	503	1	14,14,15	0.29	0	15,19,21	0.57	0
3	NAG	D	201	2	14,14,15	0.86	1 (7%)	15,19,21	1.62	5 (33%)
3	NAG	E	401	1	14,14,15	0.28	0	15,19,21	0.58	0
3	NAG	E	402	1	14,14,15	0.49	0	15,19,21	1.52	1 (6%)
3	NAG	F	301	2	14,14,15	0.28	0	15,19,21	0.57	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
3	NAG	A	501	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	502	1	-	0/6/23/26	0/1/1/1
3	NAG	A	503	1	-	0/6/23/26	0/1/1/1
3	NAG	B	301	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	B	302	2	-	0/6/23/26	0/1/1/1
3	NAG	C	501	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	502	1	-	0/6/23/26	0/1/1/1
3	NAG	C	503	1	-	0/6/23/26	0/1/1/1
3	NAG	D	201	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	E	401	1	-	0/6/23/26	0/1/1/1
3	NAG	E	402	1	-	0/6/23/26	0/1/1/1
3	NAG	F	301	2	1/1/5/7	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	NAG	C1-C2	2.44	1.55	1.52
3	D	201	NAG	C1-C2	2.74	1.56	1.52
3	A	502	NAG	C1-C2	2.76	1.56	1.52
3	C	501	NAG	C1-C2	3.21	1.56	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	NAG	C4-C3-C2	-4.21	104.85	111.02
3	B	302	NAG	C3-C4-C5	-3.21	104.56	110.22
3	A	502	NAG	O5-C1-C2	-3.20	107.02	111.47
3	D	201	NAG	O5-C1-C2	-2.61	107.84	111.47
3	D	201	NAG	O7-C7-C8	-2.55	117.42	122.06
3	C	502	NAG	O7-C7-C8	-2.53	117.45	122.06
3	A	502	NAG	O3-C3-C4	-2.51	104.90	110.36
3	A	502	NAG	C6-C5-C4	-2.34	107.53	113.00
3	C	501	NAG	O7-C7-C8	-2.16	118.13	122.06
3	A	502	NAG	O7-C7-C8	-2.13	118.18	122.06
3	A	502	NAG	C1-C2-N2	2.01	113.92	110.49
3	D	201	NAG	C2-N2-C7	2.10	126.00	122.94
3	D	201	NAG	O3-C3-C2	2.13	113.94	109.39
3	A	502	NAG	C4-C3-C2	2.35	114.47	111.02
3	D	201	NAG	C1-O5-C5	2.81	116.04	112.17
3	A	502	NAG	C1-O5-C5	3.15	116.51	112.17
3	E	402	NAG	C1-O5-C5	4.57	118.46	112.17
3	C	502	NAG	C1-C2-N2	4.84	118.76	110.49
3	B	302	NAG	C1-O5-C5	5.99	120.42	112.17
3	C	502	NAG	C1-O5-C5	9.09	124.69	112.17

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	F	301	NAG	C1
3	B	301	NAG	C1
3	A	501	NAG	C1
3	D	201	NAG	C1

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	NAG	1	0
3	B	301	NAG	2	0
3	C	501	NAG	4	0
3	C	502	NAG	2	0
3	C	503	NAG	2	0
3	D	201	NAG	1	0
3	F	301	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

### 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	319/327 (97%)	-0.07	1 (0%) 93 92	45, 61, 83, 103	2 (0%)
1	C	319/327 (97%)	0.21	10 (3%) 49 38	52, 68, 92, 138	1 (0%)
1	E	319/327 (97%)	0.10	6 (1%) 67 58	53, 70, 94, 140	1 (0%)
2	B	172/182 (94%)	0.34	8 (4%) 32 22	40, 73, 104, 128	0
2	D	172/182 (94%)	0.39	5 (2%) 52 41	43, 78, 107, 166	0
2	F	172/182 (94%)	0.34	8 (4%) 32 22	45, 71, 113, 142	0
All	All	1473/1527 (96%)	0.18	38 (2%) 56 45	40, 68, 99, 166	4 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	134	GLY	7.9
1	C	12	ASN	7.9
1	E	12	ASN	7.5
1	E	217	ASN	5.9
2	B	171	LEU	4.6
1	E	134	GLY	3.6
2	B	164	GLU	3.2
1	A	217	ASN	3.0
2	B	57	GLU	2.9
1	C	121	ILE	2.9
1	C	119	SER	2.9
2	B	29	ALA	2.7
2	B	144	CYS	2.7
2	D	29	ALA	2.7
1	C	11	SER	2.7
1	C	37	SER	2.7
1	E	136	ASN	2.7
2	F	57	GLU	2.7
2	D	145	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
2	F	172	ASN	2.6
2	D	57	GLU	2.5
2	D	148	CYS	2.5
2	F	59	THR	2.5
2	D	144	CYS	2.5
2	F	116	LEU	2.3
1	C	270	CYS	2.3
2	B	168	LEU	2.3
2	F	72	GLU	2.3
2	F	159	HIS	2.2
1	C	242	GLY	2.2
1	E	39	ASP	2.2
2	B	110	MET	2.2
2	F	60	ASN	2.1
2	B	165	GLU	2.1
2	F	123	ARG	2.1
1	C	269	ASP	2.0
1	C	167	ALA	2.0
1	E	270	CYS	2.0

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

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
3	NAG	E	402	14/15	0.56	0.65	9.35	127,143,158,164	0
3	NAG	A	501	14/15	0.88	0.17	0.60	59,69,83,87	0
3	NAG	F	301	14/15	0.78	0.29	0.55	103,117,125,129	0
3	NAG	B	301	14/15	0.85	0.15	-1.90	90,105,110,111	0
3	NAG	B	302	14/15	0.62	0.38	-	109,129,137,147	0
3	NAG	A	502	14/15	0.91	0.20	-	78,91,98,100	0
3	NAG	C	502	14/15	0.78	0.43	-	122,140,153,154	0
3	NAG	C	503	14/15	0.80	0.23	-	62,94,106,106	0
3	NAG	D	201	14/15	0.28	0.62	-	126,146,159,162	0
3	NAG	E	401	14/15	0.66	0.44	-	127,138,148,149	0
3	NAG	A	503	14/15	0.85	0.16	-	91,106,122,123	0
3	NAG	C	501	14/15	0.28	0.74	-	141,166,183,187	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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
3	NAG	E	402	14/15	0.56	0.65	9.35	127,143,158,164	0
3	NAG	A	501	14/15	0.88	0.17	0.60	59,69,83,87	0
3	NAG	F	301	14/15	0.78	0.29	0.55	103,117,125,129	0
3	NAG	B	301	14/15	0.85	0.15	-1.90	90,105,110,111	0
3	NAG	B	302	14/15	0.62	0.38	-	109,129,137,147	0
3	NAG	A	502	14/15	0.91	0.20	-	78,91,98,100	0
3	NAG	C	502	14/15	0.78	0.43	-	122,140,153,154	0
3	NAG	C	503	14/15	0.80	0.23	-	62,94,106,106	0
3	NAG	D	201	14/15	0.28	0.62	-	126,146,159,162	0
3	NAG	E	401	14/15	0.66	0.44	-	127,138,148,149	0
3	NAG	A	503	14/15	0.85	0.16	-	91,106,122,123	0
3	NAG	C	501	14/15	0.28	0.74	-	141,166,183,187	0

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

There are no such residues in this entry.