



# Full wwPDB X-ray Structure Validation Report ⓘ

May 30, 2016 – 10:42 AM EDT

PDB ID : 5HU8  
Title : The crystal structure of hemagglutinin from A/Sichuan/26221/2014 (H5N6) influenza virus  
Authors : Yang, H.; Carney, P.J.; Guo, Z.; Chang, J.C.; Stevens, J.  
Deposited on : 2016-01-27  
Resolution : 2.45 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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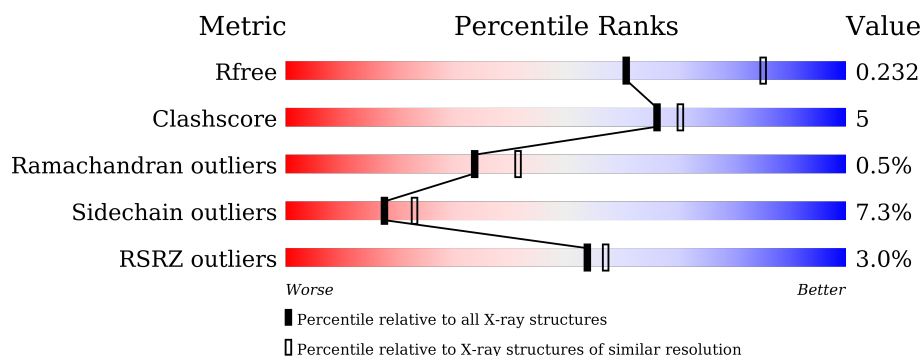
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027674  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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-20027674

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## X-RAY DIFFRACTION

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))
$R_{free}$	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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	334	<div> <div></div> <div>81%</div> <div>13%</div> <div>• •</div> </div>
1	C	334	<div> <div></div> <div>80%</div> <div>13%</div> <div>• •</div> </div>
1	E	334	<div> <div></div> <div>84%</div> <div>10%</div> <div>• •</div> </div>
2	B	181	<div> <div></div> <div>71%</div> <div>17%</div> <div>• 10%</div> </div>
2	D	181	<div> <div></div> <div>71%</div> <div>16%</div> <div>• 10%</div> </div>
2	F	181	<div> <div></div> <div>70%</div> <div>17%</div> <div>• 10%</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	C	403	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12524 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2537	1605	440	477	15			
1	C	320	Total	C	N	O	S	0	0	0
			2537	1605	440	477	15			
1	E	320	Total	C	N	O	S	0	0	0
			2537	1605	440	477	15			

- Molecule 2 is a protein called hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	162	Total	C	N	O	S	0	0	0
			1329	823	234	264	8			
2	D	162	Total	C	N	O	S	0	0	0
			1329	823	234	264	8			
2	F	162	Total	C	N	O	S	0	0	0
			1329	823	234	264	8			

- Molecule 3 is 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	A	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	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 ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			10	6	4		
4	E	1	Total	C	O	0	0
			10	6	4		
4	E	1	Total	C	O	0	0
			10	6	4		

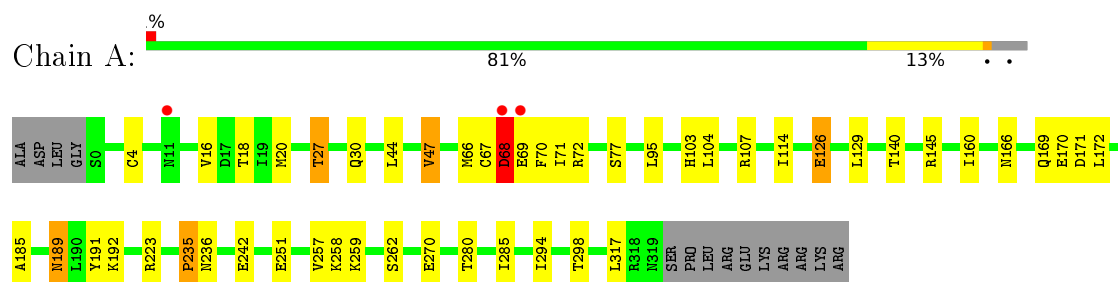
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	177	Total	O	0	0
			177	177		
5	C	154	Total	O	0	0
			154	154		
5	E	148	Total	O	0	0
			148	148		
5	B	76	Total	O	0	0
			76	76		
5	D	71	Total	O	0	0
			71	71		
5	F	72	Total	O	0	0
			72	72		

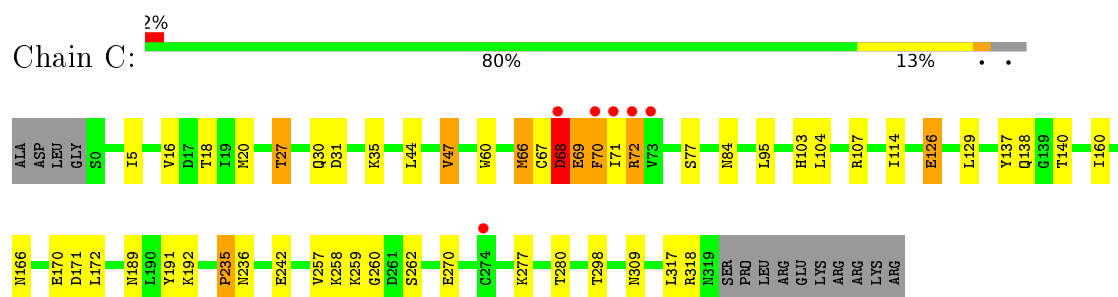
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

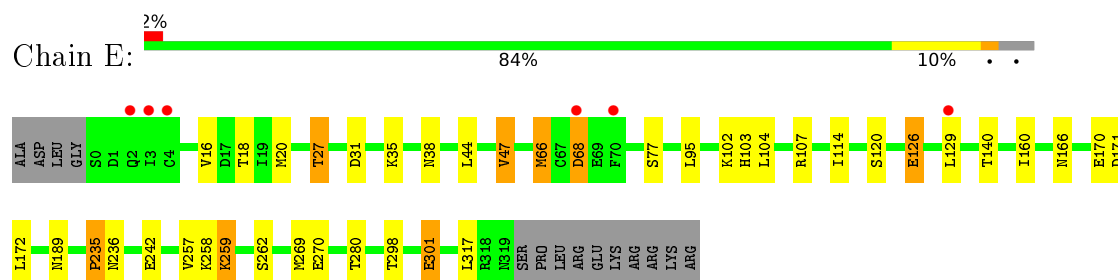
#### • Molecule 1: hemagglutinin HA1



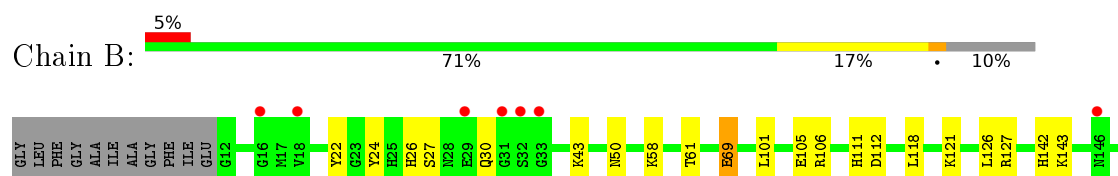
#### • Molecule 1: hemagglutinin HA1

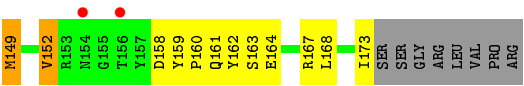


#### • Molecule 1: hemagglutinin HA1

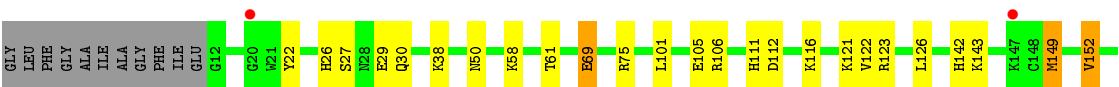


#### • Molecule 2: hemagglutinin HA2





● Molecule 2: hemagglutinin HA2



● Molecule 2: hemagglutinin HA2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.50Å 104.42Å 215.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 2.45 49.39 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.39-2.45) 99.6 (49.39-2.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.191 , 0.227 0.197 , 0.232	Depositor DCC
$R_{free}$ test set	3763 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.8	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 37.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12524	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, FUC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.76	1/2599 (0.0%)	0.86	3/3534 (0.1%)
1	C	0.69	1/2599 (0.0%)	0.82	2/3534 (0.1%)
1	E	0.69	1/2599 (0.0%)	0.85	2/3534 (0.1%)
2	B	0.74	1/1354 (0.1%)	0.79	0/1819
2	D	0.70	1/1354 (0.1%)	0.77	0/1819
2	F	0.69	1/1354 (0.1%)	0.77	0/1819
All	All	0.71	6/11859 (0.1%)	0.82	7/16059 (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	1
1	C	0	3
All	All	0	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	69	GLU	CD-OE1	8.68	1.35	1.25
2	F	69	GLU	CD-OE1	7.01	1.33	1.25
1	C	60	TRP	CB-CG	-6.31	1.38	1.50
1	E	301	GLU	CD-OE1	5.44	1.31	1.25
1	A	236	ASN	N-CA	5.36	1.57	1.46
2	D	69	GLU	CD-OE1	5.35	1.31	1.25

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	PRO	C-N-CA	-6.52	105.41	121.70
1	E	235	PRO	C-N-CA	-6.03	106.62	121.70
1	C	235	PRO	C-N-CA	-5.48	108.01	121.70
1	A	259	LYS	N-CA-C	5.45	125.72	111.00
1	E	259	LYS	N-CA-C	5.11	124.80	111.00
1	C	260	GLY	N-CA-C	5.11	125.87	113.10
1	A	223	ARG	NE-CZ-NH2	-5.09	117.75	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	72	ARG	Peptide
1	C	309	ASN	Peptide
1	C	68	ASP	Peptide
1	C	72	ARG	Peptide

## 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	2537	0	2484	22	1
1	C	2537	0	2484	29	1
1	E	2537	0	2484	21	1
2	B	1329	0	1242	17	0
2	D	1329	0	1242	17	0
2	F	1329	0	1242	19	1
3	A	56	0	49	0	0
3	C	56	0	49	1	0
3	E	56	0	49	1	0
4	A	20	0	20	0	0
4	C	20	0	20	0	0
4	E	20	0	20	0	0
5	A	177	0	0	2	0
5	B	76	0	0	5	0
5	C	154	0	0	6	0
5	D	71	0	0	4	0
5	E	148	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	72	0	0	6	0
All	All	12524	0	11385	113	2

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 5.

All (113) 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:C:84:ASN:HB3	5:C:623:HOH:O	1.58	1.03
1:E:18:THR:HG21	5:E:589:HOH:O	1.58	1.02
1:C:66:MET:HE2	5:C:638:HOH:O	1.75	0.85
2:B:105:GLU:HG3	5:B:266:HOH:O	1.81	0.80
1:C:137:TYR:O	1:C:140:THR:HG22	1.83	0.78
1:C:67:CYS:O	1:C:69:GLU:N	2.18	0.76
1:E:126:GLU:HG3	1:E:129:LEU:HD22	1.68	0.76
1:A:126:GLU:HG3	1:A:129:LEU:HD22	1.69	0.74
1:C:126:GLU:HG3	1:C:129:LEU:HD22	1.70	0.74
2:D:164:GLU:HB3	5:D:237:HOH:O	1.88	0.73
1:C:236:ASN:OD1	3:C:403:NAG:H5	1.90	0.72
1:C:68:ASP:O	1:C:70:PHE:N	2.18	0.72
2:F:22:TYR:OH	2:F:111:HIS:HD2	1.72	0.71
2:D:22:TYR:OH	2:D:111:HIS:HD2	1.74	0.71
2:F:148:CYS:SG	5:F:208:HOH:O	2.49	0.70
2:B:22:TYR:OH	2:B:111:HIS:HD2	1.74	0.70
2:B:105:GLU:OE2	2:F:106:ARG:CZ	2.41	0.68
2:B:105:GLU:OE2	2:F:106:ARG:NH1	2.28	0.66
2:D:167:ARG:HG3	5:D:205:HOH:O	1.95	0.65
2:F:27:SER:HA	5:F:206:HOH:O	1.97	0.65
1:C:166:ASN:O	1:C:235:PRO:O	2.16	0.64
1:A:67:CYS:O	1:A:69:GLU:N	2.25	0.64
1:A:18:THR:HG22	1:A:20:MET:H	1.63	0.63
1:A:166:ASN:O	1:A:235:PRO:O	2.17	0.62
1:E:166:ASN:O	1:E:235:PRO:O	2.16	0.62
2:F:29:GLU:HB2	5:F:207:HOH:O	2.00	0.62
1:C:137:TYR:O	1:C:140:THR:CG2	2.47	0.62
1:A:169:GLN:HG2	5:A:647:HOH:O	2.00	0.60
1:C:18:THR:HG22	1:C:20:MET:H	1.65	0.60
1:C:47:VAL:HG22	1:C:77:SER:HB3	1.82	0.60
1:C:68:ASP:C	1:C:70:PHE:H	2.07	0.58
1:A:47:VAL:HG22	1:A:77:SER:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:ARG:HD3	5:C:543:HOH:O	2.04	0.58
1:E:18:THR:HG22	1:E:20:MET:H	1.67	0.57
2:F:32:SER:HB3	5:F:206:HOH:O	2.04	0.57
2:F:113:SER:HB2	5:F:252:HOH:O	2.04	0.57
1:E:47:VAL:HG22	1:E:77:SER:HB3	1.86	0.56
2:F:26:HIS:HB2	2:F:149:MET:HG3	1.88	0.54
1:C:170:GLU:HG2	1:C:257:VAL:CG2	2.37	0.54
1:E:301:GLU:HB3	2:F:61:THR:HG23	1.90	0.53
1:A:103:HIS:HE1	5:A:643:HOH:O	1.91	0.53
2:D:164:GLU:HA	2:D:167:ARG:HB2	1.90	0.53
1:A:170:GLU:HG2	1:A:257:VAL:CG2	2.39	0.53
1:A:18:THR:HG21	5:B:266:HOH:O	2.08	0.52
2:B:26:HIS:HB2	2:B:149:MET:HG3	1.91	0.52
1:E:170:GLU:HG2	1:E:257:VAL:CG2	2.39	0.52
1:C:138:GLN:HG2	5:C:512:HOH:O	2.10	0.52
1:E:102:LYS:NZ	5:E:505:HOH:O	2.42	0.52
2:D:75:ARG:HD2	5:D:219:HOH:O	2.10	0.51
1:A:103:HIS:HD2	2:B:69:GLU:OE2	1.93	0.51
1:A:68:ASP:OD1	1:A:145:ARG:HD2	2.11	0.51
1:E:31:ASP:OD2	1:E:35:LYS:NZ	2.44	0.50
2:B:127:ARG:N	5:B:202:HOH:O	2.43	0.50
1:C:5:ILE:HD11	2:D:122:VAL:HG21	1.94	0.50
1:C:103:HIS:HD2	2:D:69:GLU:OE2	1.95	0.50
2:D:26:HIS:HB2	2:D:149:MET:HG3	1.94	0.49
1:C:280:THR:HG22	1:C:298:THR:HG22	1.95	0.49
2:B:159:TYR:N	2:B:160:PRO:HD2	2.29	0.48
1:A:280:THR:HG22	1:A:298:THR:HG22	1.95	0.48
2:B:106:ARG:CZ	2:D:105:GLU:OE2	2.63	0.47
1:E:280:THR:HG22	1:E:298:THR:HG22	1.97	0.47
1:C:277:LYS:HD2	5:C:639:HOH:O	2.14	0.47
1:E:66:MET:HE2	5:E:636:HOH:O	2.15	0.47
2:F:164:GLU:HG3	2:F:167:ARG:NH1	2.31	0.46
2:D:106:ARG:HH12	2:F:106:ARG:HG2	1.81	0.46
1:A:69:GLU:O	1:A:71:ILE:N	2.48	0.46
1:C:69:GLU:O	1:C:71:ILE:N	2.48	0.46
2:F:142:HIS:CD2	2:F:162:TYR:CD2	3.04	0.46
2:B:43:LYS:HB3	5:B:253:HOH:O	2.16	0.46
2:D:142:HIS:CD2	2:D:162:TYR:CD2	3.04	0.46
2:D:126:LEU:HD21	2:D:152:VAL:HG11	1.97	0.46
1:C:68:ASP:C	1:C:70:PHE:N	2.68	0.45
1:E:236:ASN:OD1	3:E:403:NAG:H5	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:ARG:HG3	5:B:202:HOH:O	2.17	0.45
2:D:38:LYS:HB3	5:D:255:HOH:O	2.16	0.45
1:C:31:ASP:OD2	1:C:35:LYS:NZ	2.50	0.45
1:C:114:ILE:HD11	1:C:172:LEU:HD11	2.00	0.44
2:F:69:GLU:HG3	5:F:246:HOH:O	2.17	0.44
2:F:126:LEU:HD21	2:F:152:VAL:HG11	1.99	0.44
2:B:106:ARG:NH1	2:D:105:GLU:OE2	2.51	0.44
1:E:114:ILE:HD11	1:E:172:LEU:HD11	1.99	0.43
1:A:191:TYR:O	1:A:192:LYS:HB3	2.19	0.43
2:B:164:GLU:OE2	2:B:167:ARG:NH1	2.47	0.43
2:F:167:ARG:NH2	2:F:168:LEU:HD21	2.33	0.43
1:E:103:HIS:HD2	2:F:69:GLU:OE2	2.01	0.43
1:E:27:THR:HB	1:E:317:LEU:H	1.83	0.43
1:C:27:THR:HB	1:C:317:LEU:H	1.84	0.43
1:A:171:ASP:OD1	1:A:235:PRO:HD3	2.19	0.42
1:A:107:ARG:HB2	1:A:262:SER:HB2	2.01	0.42
1:E:107:ARG:HB2	1:E:262:SER:HB2	2.01	0.42
1:A:4:CYS:O	2:B:24:TYR:HA	2.20	0.42
1:C:170:GLU:HG2	1:C:257:VAL:HG23	2.00	0.42
2:D:22:TYR:HH	2:D:111:HIS:HD2	1.67	0.42
2:D:169:LYS:O	2:D:169:LYS:HD2	2.20	0.42
1:C:171:ASP:OD1	1:C:235:PRO:HD3	2.19	0.42
1:C:191:TYR:O	1:C:192:LYS:HB3	2.20	0.41
1:A:27:THR:HB	1:A:317:LEU:H	1.85	0.41
5:C:584:HOH:O	2:F:75:ARG:HD2	2.19	0.41
2:B:126:LEU:HD21	2:B:152:VAL:HG11	2.02	0.41
1:A:114:ILE:HD11	1:A:172:LEU:HD11	2.02	0.41
2:D:106:ARG:NH1	2:F:105:GLU:OE2	2.53	0.41
1:E:38:ASN:C	1:E:38:ASN:OD1	2.58	0.41
1:E:160:ILE:O	1:E:242:GLU:HA	2.21	0.41
2:B:142:HIS:CD2	2:B:162:TYR:CD2	3.09	0.41
1:E:170:GLU:HG2	1:E:257:VAL:HG23	2.03	0.41
1:A:185:ALA:O	1:A:189:ASN:HB2	2.21	0.41
1:A:160:ILE:O	1:A:242:GLU:HA	2.21	0.41
2:B:118:LEU:HD23	2:B:118:LEU:HA	1.93	0.41
1:E:269:MET:HB3	1:E:270:GLU:H	1.70	0.40
1:A:285:ILE:HG12	1:A:294:ILE:HD13	2.04	0.40
1:C:160:ILE:O	1:C:242:GLU:HA	2.21	0.40
1:E:171:ASP:OD1	1:E:235:PRO:HD3	2.21	0.40
1:C:107:ARG:HB2	1:C:262:SER:HB2	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:SER:OG	2:F:165:GLU:OE1[2_564]	1.81	0.39
1:A:251:GLU:OE2	1:C:138:GLN:OE1[3_444]	2.19	0.01

## 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	318/334 (95%)	299 (94%)	17 (5%)	2 (1%)	30	35
1	C	318/334 (95%)	298 (94%)	17 (5%)	3 (1%)	21	25
1	E	318/334 (95%)	299 (94%)	18 (6%)	1 (0%)	46	57
2	B	160/181 (88%)	152 (95%)	8 (5%)	0	100	100
2	D	160/181 (88%)	151 (94%)	8 (5%)	1 (1%)	30	35
2	F	160/181 (88%)	152 (95%)	8 (5%)	0	100	100
All	All	1434/1545 (93%)	1351 (94%)	76 (5%)	7 (0%)	34	41

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	68	ASP
1	C	70	PHE
1	A	68	ASP
1	A	70	PHE
1	C	69	GLU
2	D	171	GLU
1	E	68	ASP

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	285/298 (96%)	271 (95%)	14 (5%)	31	43
1	C	285/298 (96%)	271 (95%)	14 (5%)	31	43
1	E	285/298 (96%)	272 (95%)	13 (5%)	33	46
2	B	142/155 (92%)	126 (89%)	16 (11%)	7	7
2	D	142/155 (92%)	124 (87%)	18 (13%)	5	5
2	F	142/155 (92%)	123 (87%)	19 (13%)	5	4
All	All	1281/1359 (94%)	1187 (93%)	94 (7%)	17	23

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	27	THR
1	A	30	GLN
1	A	44	LEU
1	A	47	VAL
1	A	66	MET
1	A	68	ASP
1	A	95	LEU
1	A	104	LEU
1	A	126	GLU
1	A	140	THR
1	A	189	ASN
1	A	258	LYS
1	A	270	GLU
1	C	16	VAL
1	C	27	THR
1	C	30	GLN
1	C	44	LEU
1	C	47	VAL
1	C	66	MET
1	C	72	ARG
1	C	95	LEU
1	C	104	LEU
1	C	126	GLU
1	C	189	ASN
1	C	258	LYS

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Mol	Chain	Res	Type
1	C	259	LYS
1	C	270	GLU
1	E	16	VAL
1	E	27	THR
1	E	44	LEU
1	E	47	VAL
1	E	66	MET
1	E	68	ASP
1	E	95	LEU
1	E	104	LEU
1	E	126	GLU
1	E	140	THR
1	E	189	ASN
1	E	258	LYS
1	E	259	LYS
2	B	27	SER
2	B	30	GLN
2	B	50	ASN
2	B	58	LYS
2	B	61	THR
2	B	101	LEU
2	B	112	ASP
2	B	121	LYS
2	B	143	LYS
2	B	149	MET
2	B	152	VAL
2	B	158	ASP
2	B	161	GLN
2	B	163	SER
2	B	168	LEU
2	B	173	ILE
2	D	27	SER
2	D	29	GLU
2	D	30	GLN
2	D	50	ASN
2	D	58	LYS
2	D	61	THR
2	D	101	LEU
2	D	112	ASP
2	D	116	LYS
2	D	121	LYS
2	D	123	ARG

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Mol	Chain	Res	Type
2	D	143	LYS
2	D	149	MET
2	D	152	VAL
2	D	161	GLN
2	D	163	SER
2	D	171	GLU
2	D	173	ILE
2	F	18	VAL
2	F	27	SER
2	F	29	GLU
2	F	30	GLN
2	F	43	LYS
2	F	50	ASN
2	F	58	LYS
2	F	61	THR
2	F	101	LEU
2	F	112	ASP
2	F	121	LYS
2	F	123	ARG
2	F	143	LYS
2	F	149	MET
2	F	152	VAL
2	F	158	ASP
2	F	161	GLN
2	F	163	SER
2	F	173	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	HIS
1	A	146	ASN
1	A	220	ASN
1	A	222	GLN
1	C	103	HIS
1	C	146	ASN
1	C	220	ASN
1	C	222	GLN
1	E	103	HIS
1	E	110	HIS
1	E	146	ASN
1	E	220	ASN

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Mol	Chain	Res	Type
2	B	111	HIS
2	B	125	GLN
2	B	142	HIS
2	B	146	ASN
2	D	111	HIS
2	D	125	GLN
2	D	142	HIS
2	D	146	ASN
2	F	111	HIS
2	F	125	GLN
2	F	142	HIS
2	F	146	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

18 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	401	1,4	14,14,15	0.57	0	15,19,21	1.68	5 (33%)
4	FUC	A	402	3	10,10,11	0.72	0	13,14,16	1.73	4 (30%)
3	NAG	A	403	1,3,4	14,14,15	0.86	1 (7%)	15,19,21	1.38	1 (6%)
3	NAG	A	404	3	14,14,15	0.71	0	15,19,21	1.57	2 (13%)
4	FUC	A	405	3	10,10,11	0.92	0	13,14,16	1.41	2 (15%)
3	NAG	A	406	1	14,14,15	1.25	2 (14%)	15,19,21	2.45	5 (33%)
3	NAG	C	401	1,4	14,14,15	0.85	0	15,19,21	1.22	2 (13%)
4	FUC	C	402	3	10,10,11	0.80	0	13,14,16	2.17	4 (30%)
3	NAG	C	403	1,3,4	14,14,15	0.62	0	15,19,21	1.43	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	C	404	3	14,14,15	0.70	0	15,19,21	1.85	3 (20%)
4	FUC	C	405	3	10,10,11	0.85	0	13,14,16	1.45	3 (23%)
3	NAG	C	406	1	14,14,15	0.68	0	15,19,21	1.66	3 (20%)
3	NAG	E	401	1,4	14,14,15	0.87	1 (7%)	15,19,21	1.79	3 (20%)
4	FUC	E	402	3	10,10,11	0.64	0	13,14,16	0.86	0
3	NAG	E	403	1,3,4	14,14,15	0.87	1 (7%)	15,19,21	1.62	4 (26%)
3	NAG	E	404	3	14,14,15	0.92	1 (7%)	15,19,21	1.81	3 (20%)
4	FUC	E	405	3	10,10,11	0.73	0	13,14,16	1.06	1 (7%)
3	NAG	E	406	1	14,14,15	0.88	0	15,19,21	1.68	3 (20%)

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	1,4	-	0/6/23/26	0/1/1/1
4	FUC	A	402	3	-	0/0/17/20	0/1/1/1
3	NAG	A	403	1,3,4	-	0/6/23/26	0/1/1/1
3	NAG	A	404	3	-	0/6/23/26	0/1/1/1
4	FUC	A	405	3	-	0/0/17/20	0/1/1/1
3	NAG	A	406	1	-	0/6/23/26	0/1/1/1
3	NAG	C	401	1,4	-	0/6/23/26	0/1/1/1
4	FUC	C	402	3	-	0/0/17/20	0/1/1/1
3	NAG	C	403	1,3,4	-	0/6/23/26	0/1/1/1
3	NAG	C	404	3	-	0/6/23/26	0/1/1/1
4	FUC	C	405	3	-	0/0/17/20	0/1/1/1
3	NAG	C	406	1	-	0/6/23/26	0/1/1/1
3	NAG	E	401	1,4	-	0/6/23/26	0/1/1/1
4	FUC	E	402	3	-	0/0/17/20	0/1/1/1
3	NAG	E	403	1,3,4	-	0/6/23/26	0/1/1/1
3	NAG	E	404	3	-	0/6/23/26	0/1/1/1
4	FUC	E	405	3	-	0/0/17/20	0/1/1/1
3	NAG	E	406	1	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	403	NAG	O5-C1	-2.25	1.40	1.43
3	A	403	NAG	O5-C1	-2.25	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	404	NAG	C4-C5	2.20	1.57	1.53
3	A	406	NAG	C2-N2	2.58	1.50	1.46
3	E	401	NAG	C1-C2	2.60	1.56	1.52
3	A	406	NAG	C1-C2	2.75	1.56	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	406	NAG	O7-C7-C8	-4.50	113.78	122.07
3	A	404	NAG	O5-C5-C4	-4.26	103.08	110.13
3	E	401	NAG	C3-C4-C5	-3.68	103.66	110.23
3	C	406	NAG	O5-C5-C4	-3.54	104.28	110.13
3	A	404	NAG	C1-O5-C5	-3.18	107.47	112.14
3	C	406	NAG	C3-C4-C5	-3.12	104.66	110.23
3	A	401	NAG	C3-C4-C5	-3.04	104.80	110.23
4	A	402	FUC	C1-C2-C3	-2.80	106.16	109.55
3	E	403	NAG	O4-C4-C5	-2.62	102.32	109.23
3	A	406	NAG	O5-C5-C4	-2.51	105.97	110.13
3	E	404	NAG	C1-O5-C5	-2.47	108.51	112.14
4	A	402	FUC	O5-C1-C2	-2.14	107.48	110.89
3	E	403	NAG	C4-C3-C2	-2.07	108.13	111.34
3	C	404	NAG	C4-C3-C2	2.01	114.46	111.34
4	C	405	FUC	O4-C4-C5	2.10	114.46	109.67
3	C	403	NAG	C2-N2-C7	2.10	125.84	123.11
3	C	401	NAG	C1-O5-C5	2.11	115.24	112.14
4	E	405	FUC	C3-C4-C5	2.11	112.81	109.66
4	C	402	FUC	C2-C3-C4	2.18	114.85	111.05
3	A	401	NAG	O5-C5-C6	2.18	112.00	107.34
3	A	401	NAG	O3-C3-C2	2.29	114.27	109.37
4	A	405	FUC	O5-C5-C6	2.33	110.45	106.28
3	E	406	NAG	C2-N2-C7	2.34	126.15	123.11
3	C	403	NAG	O5-C5-C4	2.35	114.03	110.13
4	A	402	FUC	C3-C4-C5	2.41	113.26	109.66
3	A	401	NAG	O4-C4-C5	2.48	115.77	109.23
3	E	403	NAG	O5-C5-C6	2.53	112.75	107.34
4	C	405	FUC	C1-C2-C3	2.54	112.63	109.55
3	E	404	NAG	O5-C5-C4	2.56	114.37	110.13
3	E	401	NAG	C1-O5-C5	2.59	115.95	112.14
3	E	406	NAG	O4-C4-C5	2.66	116.23	109.23
4	A	405	FUC	C3-C4-C5	2.81	113.86	109.66
4	A	402	FUC	O2-C2-C1	2.82	114.89	109.23
3	C	401	NAG	C3-C4-C5	2.86	115.33	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	NAG	C1-O5-C5	2.88	116.38	112.14
3	E	403	NAG	O3-C3-C4	2.92	116.95	110.36
4	C	405	FUC	O5-C5-C6	2.94	111.55	106.28
3	A	406	NAG	C4-C3-C2	3.07	116.10	111.34
3	C	404	NAG	O5-C5-C6	3.28	114.36	107.34
3	C	406	NAG	O4-C4-C5	3.36	118.07	109.23
3	E	406	NAG	C4-C3-C2	3.37	116.58	111.34
3	A	403	NAG	O3-C3-C4	3.42	118.07	110.36
3	C	403	NAG	C1-O5-C5	3.50	117.29	112.14
3	A	406	NAG	O7-C7-N2	3.66	129.30	121.84
3	E	401	NAG	O5-C5-C6	3.67	115.19	107.34
4	C	402	FUC	C1-C2-C3	3.87	114.24	109.55
4	C	402	FUC	C3-C4-C5	3.92	115.52	109.66
4	C	402	FUC	O5-C5-C4	4.14	116.74	109.58
3	C	404	NAG	C1-O5-C5	4.51	118.77	112.14
3	E	404	NAG	C3-C4-C5	4.91	118.98	110.23
3	A	406	NAG	C2-N2-C7	5.29	129.99	123.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	403	NAG	1	0
3	E	403	NAG	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	A	401	1,4	14,14,15	0.57	0	15,19,21	1.68	5 (33%)
4	FUC	A	402	3	10,10,11	0.72	0	13,14,16	1.73	4 (30%)
3	NAG	A	403	1,3,4	14,14,15	0.86	1 (7%)	15,19,21	1.38	1 (6%)
3	NAG	A	404	3	14,14,15	0.71	0	15,19,21	1.57	2 (13%)
4	FUC	A	405	3	10,10,11	0.92	0	13,14,16	1.41	2 (15%)
3	NAG	A	406	1	14,14,15	1.25	2 (14%)	15,19,21	2.45	5 (33%)
3	NAG	C	401	1,4	14,14,15	0.85	0	15,19,21	1.22	2 (13%)
4	FUC	C	402	3	10,10,11	0.80	0	13,14,16	2.17	4 (30%)
3	NAG	C	403	1,3,4	14,14,15	0.62	0	15,19,21	1.43	3 (20%)
3	NAG	C	404	3	14,14,15	0.70	0	15,19,21	1.85	3 (20%)
4	FUC	C	405	3	10,10,11	0.85	0	13,14,16	1.45	3 (23%)
3	NAG	C	406	1	14,14,15	0.68	0	15,19,21	1.66	3 (20%)
3	NAG	E	401	1,4	14,14,15	0.87	1 (7%)	15,19,21	1.79	3 (20%)
4	FUC	E	402	3	10,10,11	0.64	0	13,14,16	0.86	0
3	NAG	E	403	1,3,4	14,14,15	0.87	1 (7%)	15,19,21	1.62	4 (26%)
3	NAG	E	404	3	14,14,15	0.92	1 (7%)	15,19,21	1.81	3 (20%)
4	FUC	E	405	3	10,10,11	0.73	0	13,14,16	1.06	1 (7%)
3	NAG	E	406	1	14,14,15	0.88	0	15,19,21	1.68	3 (20%)

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	1,4	-	0/6/23/26	0/1/1/1
4	FUC	A	402	3	-	0/0/17/20	0/1/1/1
3	NAG	A	403	1,3,4	-	0/6/23/26	0/1/1/1
3	NAG	A	404	3	-	0/6/23/26	0/1/1/1
4	FUC	A	405	3	-	0/0/17/20	0/1/1/1
3	NAG	A	406	1	-	0/6/23/26	0/1/1/1
3	NAG	C	401	1,4	-	0/6/23/26	0/1/1/1
4	FUC	C	402	3	-	0/0/17/20	0/1/1/1
3	NAG	C	403	1,3,4	-	0/6/23/26	0/1/1/1
3	NAG	C	404	3	-	0/6/23/26	0/1/1/1
4	FUC	C	405	3	-	0/0/17/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	406	1	-	0/6/23/26	0/1/1/1
3	NAG	E	401	1,4	-	0/6/23/26	0/1/1/1
4	FUC	E	402	3	-	0/0/17/20	0/1/1/1
3	NAG	E	403	1,3,4	-	0/6/23/26	0/1/1/1
3	NAG	E	404	3	-	0/6/23/26	0/1/1/1
4	FUC	E	405	3	-	0/0/17/20	0/1/1/1
3	NAG	E	406	1	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	403	NAG	O5-C1	-2.25	1.40	1.43
3	A	403	NAG	O5-C1	-2.25	1.40	1.43
3	E	404	NAG	C4-C5	2.20	1.57	1.53
3	A	406	NAG	C2-N2	2.58	1.50	1.46
3	E	401	NAG	C1-C2	2.60	1.56	1.52
3	A	406	NAG	C1-C2	2.75	1.56	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	406	NAG	O7-C7-C8	-4.50	113.78	122.07
3	A	404	NAG	O5-C5-C4	-4.26	103.08	110.13
3	E	401	NAG	C3-C4-C5	-3.68	103.66	110.23
3	C	406	NAG	O5-C5-C4	-3.54	104.28	110.13
3	A	404	NAG	C1-O5-C5	-3.18	107.47	112.14
3	C	406	NAG	C3-C4-C5	-3.12	104.66	110.23
3	A	401	NAG	C3-C4-C5	-3.04	104.80	110.23
4	A	402	FUC	C1-C2-C3	-2.80	106.16	109.55
3	E	403	NAG	O4-C4-C5	-2.62	102.32	109.23
3	A	406	NAG	O5-C5-C4	-2.51	105.97	110.13
3	E	404	NAG	C1-O5-C5	-2.47	108.51	112.14
4	A	402	FUC	O5-C1-C2	-2.14	107.48	110.89
3	E	403	NAG	C4-C3-C2	-2.07	108.13	111.34
3	C	404	NAG	C4-C3-C2	2.01	114.46	111.34
4	C	405	FUC	O4-C4-C5	2.10	114.46	109.67
3	C	403	NAG	C2-N2-C7	2.10	125.84	123.11
3	C	401	NAG	C1-O5-C5	2.11	115.24	112.14
4	E	405	FUC	C3-C4-C5	2.11	112.81	109.66
4	C	402	FUC	C2-C3-C4	2.18	114.85	111.05
3	A	401	NAG	O5-C5-C6	2.18	112.00	107.34
3	A	401	NAG	O3-C3-C2	2.29	114.27	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	405	FUC	O5-C5-C6	2.33	110.45	106.28
3	E	406	NAG	C2-N2-C7	2.34	126.15	123.11
3	C	403	NAG	O5-C5-C4	2.35	114.03	110.13
4	A	402	FUC	C3-C4-C5	2.41	113.26	109.66
3	A	401	NAG	O4-C4-C5	2.48	115.77	109.23
3	E	403	NAG	O5-C5-C6	2.53	112.75	107.34
4	C	405	FUC	C1-C2-C3	2.54	112.63	109.55
3	E	404	NAG	O5-C5-C4	2.56	114.37	110.13
3	E	401	NAG	C1-O5-C5	2.59	115.95	112.14
3	E	406	NAG	O4-C4-C5	2.66	116.23	109.23
4	A	405	FUC	C3-C4-C5	2.81	113.86	109.66
4	A	402	FUC	O2-C2-C1	2.82	114.89	109.23
3	C	401	NAG	C3-C4-C5	2.86	115.33	110.23
3	A	401	NAG	C1-O5-C5	2.88	116.38	112.14
3	E	403	NAG	O3-C3-C4	2.92	116.95	110.36
4	C	405	FUC	O5-C5-C6	2.94	111.55	106.28
3	A	406	NAG	C4-C3-C2	3.07	116.10	111.34
3	C	404	NAG	O5-C5-C6	3.28	114.36	107.34
3	C	406	NAG	O4-C4-C5	3.36	118.07	109.23
3	E	406	NAG	C4-C3-C2	3.37	116.58	111.34
3	A	403	NAG	O3-C3-C4	3.42	118.07	110.36
3	C	403	NAG	C1-O5-C5	3.50	117.29	112.14
3	A	406	NAG	O7-C7-N2	3.66	129.30	121.84
3	E	401	NAG	O5-C5-C6	3.67	115.19	107.34
4	C	402	FUC	C1-C2-C3	3.87	114.24	109.55
4	C	402	FUC	C3-C4-C5	3.92	115.52	109.66
4	C	402	FUC	O5-C5-C4	4.14	116.74	109.58
3	C	404	NAG	C1-O5-C5	4.51	118.77	112.14
3	E	404	NAG	C3-C4-C5	4.91	118.98	110.23
3	A	406	NAG	C2-N2-C7	5.29	129.99	123.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	403	NAG	1	0
3	E	403	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	320/334 (95%)	-0.35	3 (0%) 85 87	26, 42, 74, 131	0
1	C	320/334 (95%)	-0.25	6 (1%) 70 72	32, 50, 79, 163	0
1	E	320/334 (95%)	-0.31	6 (1%) 70 72	28, 51, 81, 169	0
2	B	162/181 (89%)	0.12	9 (5%) 28 30	29, 63, 96, 120	0
2	D	162/181 (89%)	0.12	3 (1%) 70 72	28, 74, 122, 159	0
2	F	162/181 (89%)	0.31	16 (9%) 9 9	31, 76, 111, 139	0
All	All	1446/1545 (93%)	-0.14	43 (2%) 54 57	26, 52, 101, 169	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	ASP	8.0
1	C	71	ILE	7.6
2	B	31	GLY	5.7
1	C	72	ARG	5.5
1	E	68	ASP	5.0
2	B	18	VAL	4.7
1	C	70	PHE	4.4
1	E	2	GLN	4.0
1	C	68	ASP	4.0
2	B	33	GLY	3.6
2	F	140	PHE	3.6
1	E	4	CYS	3.5
2	F	138	PHE	3.5
1	E	70	PHE	3.5
2	B	32	SER	3.4
2	F	27	SER	3.3
2	F	152	VAL	3.2
2	F	133	LEU	3.2
1	C	73	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
2	F	119	TYR	2.9
2	B	146	ASN	2.8
2	F	139	GLU	2.7
2	F	173	ILE	2.7
2	F	131	LYS	2.6
2	F	34	TYR	2.5
2	B	16	GLY	2.5
2	F	134	GLY	2.5
1	C	274	CYS	2.4
2	B	156	THR	2.3
2	F	142	HIS	2.3
1	A	69	GLU	2.2
2	D	173	ILE	2.2
2	F	150	GLU	2.2
2	B	154	ASN	2.2
1	E	129	LEU	2.2
2	B	29	GLU	2.1
2	F	23	GLY	2.1
2	F	166	ALA	2.1
1	E	3	ILE	2.1
2	F	18	VAL	2.0
2	D	147	LYS	2.0
1	A	11	ASN	2.0
2	D	20	GLY	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	C	403	14/15	0.91	0.18	4.92	74,80,101,111	0
3	NAG	E	403	14/15	0.94	0.11	-0.85	58,64,88,117	0
4	FUC	A	405	10/11	0.87	0.39	-	91,110,116,119	0
4	FUC	C	402	10/11	0.56	0.54	-	142,156,169,172	0
3	NAG	A	401	14/15	0.88	0.18	-	97,106,113,117	0
4	FUC	C	405	10/11	0.83	0.51	-	117,128,140,143	0
3	NAG	A	404	14/15	0.93	0.26	-	88,101,114,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	C	401	14/15	0.73	0.27	-	103,119,137,146	0
3	NAG	A	406	14/15	0.81	0.16	-	91,104,109,114	0
3	NAG	E	404	14/15	0.85	0.16	-	82,104,116,118	0
3	NAG	C	406	14/15	0.82	0.27	-	89,102,105,107	0
3	NAG	E	406	14/15	0.67	0.25	-	89,112,132,136	0
3	NAG	E	401	14/15	0.78	0.13	-	100,108,130,146	0
3	NAG	C	404	14/15	0.81	0.33	-	83,113,124,128	0
4	FUC	E	405	10/11	0.86	0.26	-	103,128,131,141	0
4	FUC	A	402	10/11	0.82	0.37	-	95,113,116,116	0
3	NAG	A	403	14/15	0.91	0.14	-	45,59,91,108	0
4	FUC	E	402	10/11	0.73	0.27	-	121,147,156,161	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	C	403	14/15	0.91	0.18	4.92	74,80,101,111	0
3	NAG	E	403	14/15	0.94	0.11	-0.85	58,64,88,117	0
4	FUC	A	402	10/11	0.82	0.37	-	95,113,116,116	0
4	FUC	A	405	10/11	0.87	0.39	-	91,110,116,119	0
3	NAG	E	404	14/15	0.85	0.16	-	82,104,116,118	0
3	NAG	A	401	14/15	0.88	0.18	-	97,106,113,117	0
4	FUC	C	405	10/11	0.83	0.51	-	117,128,140,143	0
4	FUC	E	405	10/11	0.86	0.26	-	103,128,131,141	0
3	NAG	C	401	14/15	0.73	0.27	-	103,119,137,146	0
3	NAG	A	406	14/15	0.81	0.16	-	91,104,109,114	0
3	NAG	C	406	14/15	0.82	0.27	-	89,102,105,107	0
3	NAG	E	406	14/15	0.67	0.25	-	89,112,132,136	0
3	NAG	E	401	14/15	0.78	0.13	-	100,108,130,146	0
4	FUC	E	402	10/11	0.73	0.27	-	121,147,156,161	0
3	NAG	A	404	14/15	0.93	0.26	-	88,101,114,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	FUC	C	402	10/11	0.56	0.54	-	142,156,169,172	0
3	NAG	A	403	14/15	0.91	0.14	-	45,59,91,108	0
3	NAG	C	404	14/15	0.81	0.33	-	83,113,124,128	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.