



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:41 PM GMT

PDB ID : 4FNK  
Title : Crystal structure of the A/Hong Kong/1/1968 (H3N2) influenza virus hemagglutinin  
Authors : Ekiert, D.C.; Wilson, I.A.  
Deposited on : 2012-06-19  
Resolution : 1.90 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

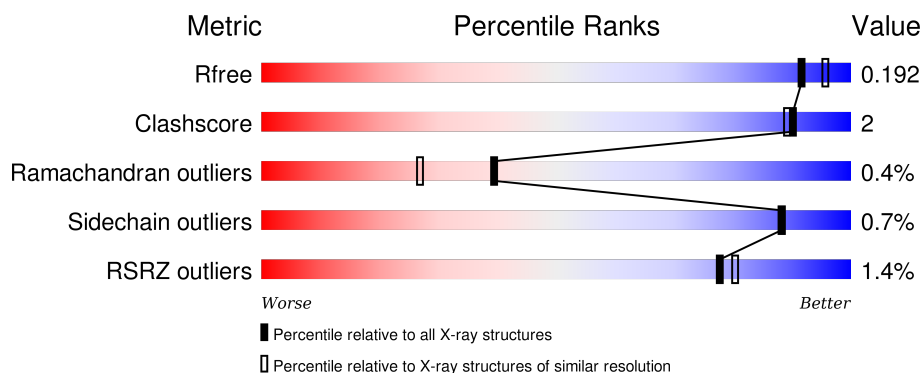
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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>%</div> <div> <div></div> <div>92%</div> <div>7%</div> <div>.</div> </div> </div>
1	C	323	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>.</div> </div> </div>
1	E	323	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>6%</div> <div>.</div> </div> </div>
2	B	174	<div> <div>2%</div> <div> <div></div> <div>95%</div> <div>.</div> <div>..</div> </div> </div>
2	D	174	<div> <div>%</div> <div> <div></div> <div>95%</div> <div>.</div> <div>...</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	174	<div> <div></div> <div>94%</div> <div>...</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	401	-	-	-	X
3	NAG	A	402	-	-	-	X
3	NAG	A	403	-	-	-	X
3	NAG	E	502	-	-	-	X
3	NAG	F	201	-	-	-	X
5	NAG	A	408	-	-	-	X
5	NAG	C	501	-	-	-	X
5	NAG	C	503	-	-	-	X
5	NAG	C	508	-	-	-	X
5	NAG	E	508	-	-	-	X
8	GOL	C	510	-	-	-	X
9	NAG	E	503	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14165 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	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	C	317	Total	C	N	O	S	0	12	0
			2546	1592	451	489	14			
1	E	318	Total	C	N	O	S	0	12	0
			2558	1602	453	489	14			

There are 12 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
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
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

- 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	7	0
			1446	901	251	287	7			
2	D	171	Total	C	N	O	S	0	8	0
			1445	898	251	289	7			
2	F	171	Total	C	N	O	S	0	9	0
			1452	905	251	289	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
D	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
F	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7

- Molecule 3 is SUGAR (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	B	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		

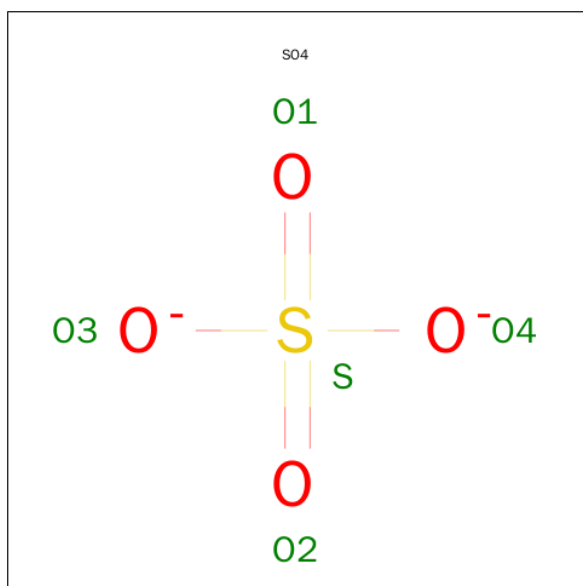
- Molecule 4 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 6 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

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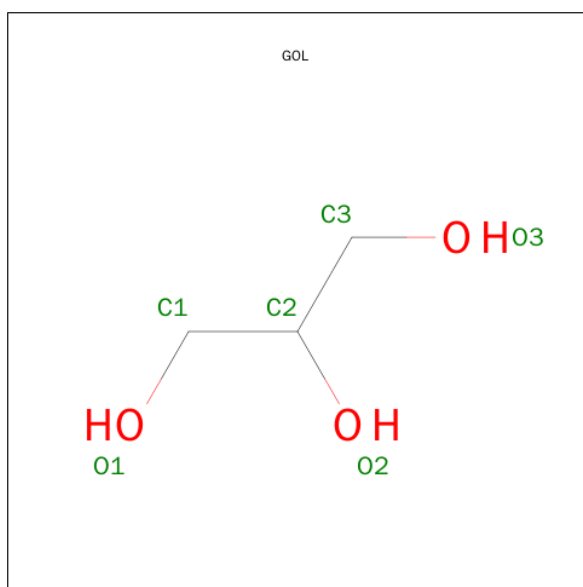
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			6	3	3		
8	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	E	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	345	Total 345	O 345	0	0
10	B	229	Total 229	O 229	0	0
10	C	319	Total 319	O 319	0	0
10	D	224	Total 224	O 224	0	0
10	E	365	Total 365	O 365	0	0
10	F	225	Total 225	O 225	0	0



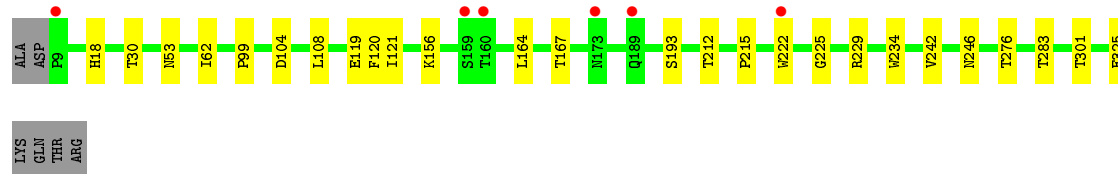
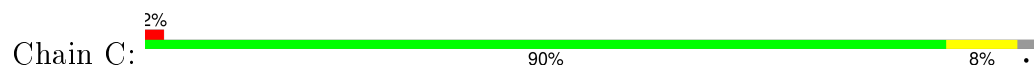
### 3 Residue-property plots [i](#)

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

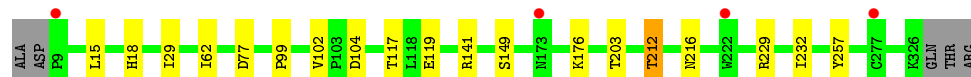
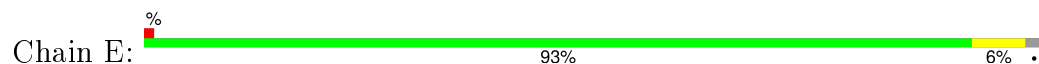
- Molecule 1: Hemagglutinin HA1 chain



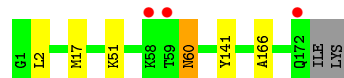
- Molecule 1: Hemagglutinin HA1 chain



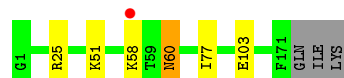
- Molecule 1: Hemagglutinin HA1 chain



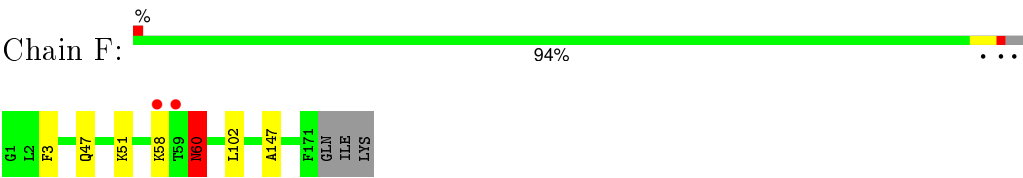
- Molecule 2: Hemagglutinin HA2 chain



- Molecule 2: Hemagglutinin HA2 chain



● Molecule 2: Hemagglutinin HA2 chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.15Å 151.46Å 347.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.06 – 1.90 43.06 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (43.06-1.90) 99.2 (43.06-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 1.89Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.162 , 0.189 0.167 , 0.192	Depositor DCC
$R_{free}$ test set	10833 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.6	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 56.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 215400 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14165	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, GOL, BMA, NAG, SO4

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	0.63	1/2612 (0.0%)	0.69	0/3558
1	C	0.64	0/2605	0.70	2/3549 (0.1%)
1	E	0.63	0/2617	0.68	1/3564 (0.0%)
2	B	0.75	0/1470	0.71	0/1975
2	D	0.73	0/1469	0.73	0/1974
2	F	0.73	0/1476	0.71	0/1984
All	All	0.67	1/12249 (0.0%)	0.70	3/16604 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	323	VAL	CB-CG2	-6.21	1.39	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	104	ASP	CB-CG-OD1	5.39	123.15	118.30
1	E	104	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	C	104	ASP	CB-CG-OD2	-5.03	113.78	118.30

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	2553	0	2489	15	0
1	C	2546	0	2481	15	0
1	E	2558	0	2501	16	0
2	B	1446	0	1370	6	0
2	D	1445	0	1360	5	0
2	F	1452	0	1373	6	0
3	A	42	0	39	0	0
3	B	14	0	13	0	0
3	E	28	0	26	0	0
3	F	14	0	13	1	0
4	A	50	0	43	0	0
5	A	28	0	25	0	0
5	C	84	0	75	1	0
5	D	28	0	25	0	0
5	E	28	0	25	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
6	D	10	0	0	1	0
6	E	5	0	0	0	0
6	F	5	0	0	0	0
7	C	39	0	34	0	0
8	C	6	0	8	0	0
8	E	6	0	8	0	0
9	E	61	0	52	2	0
10	A	345	0	0	2	0
10	B	229	0	0	0	0
10	C	319	0	0	1	0
10	D	224	0	0	1	0
10	E	365	0	0	0	0
10	F	225	0	0	0	0
All	All	14165	0	11960	56	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 2.

All (56) 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:117:THR:OG1	1:E:119[B]:GLU:CG	2.28	0.82
1:E:117:THR:OG1	1:E:119[B]:GLU:HG3	1.78	0.81
1:C:325:GLU:OE1	10:C:848:HOH:O	2.06	0.72
1:E:203:THR:OG1	1:E:212:THR:HG22	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:LYS:HD3	1:A:275[B]:ASP:OD2	1.96	0.65
1:E:203:THR:HG23	1:E:212:THR:HG23	1.79	0.65
9:E:505:BMA:C2	9:E:506:MAN:H5	2.31	0.61
1:E:117:THR:OG1	1:E:119[B]:GLU:HG2	2.00	0.60
2:F:47:GLN:O	2:F:51[B]:LYS:HG3	2.04	0.57
1:C:156:LYS:HE3	1:C:193:SER:O	2.04	0.57
1:C:121:ILE:N	1:C:121:ILE:HD12	2.20	0.55
1:A:29:ILE:HG22	2:F:51[B]:LYS:HD2	1.89	0.55
2:B:51[B]:LYS:CD	1:C:30:THR:HG22	2.37	0.55
2:F:60:ASN:N	2:F:60:ASN:HD22	2.06	0.53
1:A:222:TRP:CZ2	1:A:225:GLY:HA2	2.44	0.53
1:A:276:THR:O	1:A:276:THR:HG23	2.09	0.52
2:B:51[B]:LYS:HG2	1:C:30:THR:HG22	1.92	0.52
2:D:51[B]:LYS:HG2	1:E:29:ILE:HG22	1.92	0.52
2:F:147:ALA:O	3:F:201:NAG:O6	2.30	0.50
1:A:216:ASN:HB3	1:E:212:THR:HG21	1.95	0.49
9:E:505:BMA:H2	9:E:506:MAN:H5	1.93	0.49
1:E:141[B]:ARG:HH22	1:E:149:SER:HB3	1.77	0.49
1:A:50:LYS:CD	1:A:275[B]:ASP:OD2	2.60	0.49
1:A:216:ASN:ND2	1:E:212:THR:HB	2.29	0.48
1:A:222:TRP:CE2	1:A:225:GLY:HA2	2.49	0.48
1:C:120:PHE:C	1:C:121:ILE:HD12	2.35	0.47
2:D:77[B]:ILE:HG22	10:D:349:HOH:O	2.14	0.47
1:A:98:TYR:HH	1:A:228[B]:SER:HB2	1.78	0.46
2:D:25:ARG:NH2	6:D:203:SO4:O2	2.32	0.46
1:A:208:ARG:HB2	10:A:775:HOH:O	2.16	0.45
1:A:49:GLY:HA2	1:A:285:ASN:O	2.16	0.45
2:B:2:LEU:HB3	2:F:3:PHE:CZ	2.51	0.45
1:C:283:THR:HG22	1:C:301:THR:HG22	1.99	0.45
2:B:141:TYR:O	2:B:166:ALA:HA	2.17	0.44
1:C:164:LEU:O	1:C:246:ASN:HA	2.18	0.44
1:C:108:LEU:HB2	1:C:234[A]:TRP:CZ3	2.52	0.44
1:A:52:CYS:HB2	10:A:582:HOH:O	2.19	0.43
1:E:176:LYS:HE2	1:E:257:TYR:CE1	2.54	0.43
1:C:99:PRO:HB2	1:C:229:ARG:HD3	2.01	0.43
1:C:119:GLU:HB3	5:C:503:NAG:H62	2.01	0.42
1:C:167[A]:THR:OG1	1:C:242:VAL:CG1	2.68	0.42
1:C:212:THR:HB	1:E:216:ASN:CG	2.40	0.42
1:E:99:PRO:HB2	1:E:229:ARG:HD3	2.01	0.42
1:A:274[B]:ILE:O	1:A:275[B]:ASP:OD1	2.38	0.42
1:E:29:ILE:HD11	2:F:102:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:ASN:HD22	2:B:60:ASN:N	2.18	0.42
1:C:222:TRP:NE1	1:C:225:GLY:HA2	2.34	0.41
1:A:102:VAL:HG22	1:A:232:ILE:HB	2.02	0.41
1:C:53:ASN:HD21	1:C:276:THR:HG22	1.84	0.41
2:B:17[B]:MET:O	2:B:17[B]:MET:HG3	2.20	0.41
2:D:51[A]:LYS:HG3	2:D:103:GLU:OE1	2.20	0.41
1:E:77:ASP:OD2	1:E:141[B]:ARG:NH1	2.52	0.41
1:E:15:LEU:N	1:E:15:LEU:HD22	2.35	0.41
2:D:60:ASN:N	2:D:60:ASN:HD22	2.19	0.40
1:A:98:TYR:CZ	1:A:226:LEU:HD13	2.57	0.40
1:E:102:VAL:HG22	1:E:232:ILE:HB	2.03	0.40

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	328/323 (102%)	321 (98%)	6 (2%)	1 (0%)	46	35
1	C	327/323 (101%)	320 (98%)	6 (2%)	1 (0%)	46	35
1	E	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	46	35
2	B	177/174 (102%)	170 (96%)	7 (4%)	0	100	100
2	D	177/174 (102%)	168 (95%)	8 (4%)	1 (1%)	30	17
2	F	178/174 (102%)	168 (94%)	8 (4%)	2 (1%)	17	6
All	All	1515/1491 (102%)	1469 (97%)	40 (3%)	6 (0%)	39	27

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	58	LYS

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Mol	Chain	Res	Type
2	F	58	LYS
2	F	60	ASN
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	291/283 (103%)	289 (99%)	2 (1%)	88	88
1	C	290/283 (102%)	288 (99%)	2 (1%)	88	88
1	E	291/283 (103%)	289 (99%)	2 (1%)	88	88
2	B	153/148 (103%)	152 (99%)	1 (1%)	88	88
2	D	153/148 (103%)	152 (99%)	1 (1%)	88	88
2	F	154/148 (104%)	153 (99%)	1 (1%)	90	90
All	All	1332/1293 (103%)	1323 (99%)	9 (1%)	88	88

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	53	ASN
2	B	60	ASN
1	C	18	HIS
1	C	215	PRO
2	D	60	ASN
1	E	18	HIS
1	E	212	THR
2	F	60	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	53	ASN
1	A	75	HIS
1	A	171	ASN
2	B	53	ASN
2	B	60	ASN
1	C	54	ASN
1	C	75	HIS
1	C	171	ASN
2	D	53	ASN
2	D	60	ASN
1	E	54	ASN
2	F	27	GLN
2	F	53	ASN
2	F	60	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

24 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	A	404	1,4	14,14,15	0.78	0	15,19,21	1.24	1 (6%)
4	NAG	A	405	4	14,14,15	0.61	0	15,19,21	0.87	0
4	BMA	A	406	4	11,11,12	0.72	0	14,15,17	0.98	1 (7%)
4	MAN	A	407	4	11,11,12	0.57	0	14,15,17	0.78	0
5	NAG	A	408	1,5	14,14,15	0.78	0	15,19,21	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	A	409	5	14,14,15	0.55	0	15,19,21	0.97	1 (6%)
5	NAG	C	501	1,5	14,14,15	0.56	0	15,19,21	1.20	2 (13%)
5	NAG	C	502	5	14,14,15	0.55	0	15,19,21	1.47	2 (13%)
5	NAG	C	503	1,5	14,14,15	0.59	0	15,19,21	1.02	1 (6%)
5	NAG	C	504	5	14,14,15	0.47	0	15,19,21	1.03	1 (6%)
7	NAG	C	505	1,7	14,14,15	1.04	0	15,19,21	1.53	3 (20%)
7	NAG	C	506	7	14,14,15	0.65	0	15,19,21	1.02	0
7	BMA	C	507	7	11,11,12	0.56	0	14,15,17	1.13	1 (7%)
5	NAG	C	508	1,5	14,14,15	0.76	0	15,19,21	1.13	1 (6%)
5	NAG	C	509	5	14,14,15	0.45	0	15,19,21	1.03	1 (6%)
5	NAG	D	201	2,5	14,14,15	0.59	0	15,19,21	1.36	1 (6%)
5	NAG	D	202	5	14,14,15	0.54	0	15,19,21	0.98	1 (6%)
9	NAG	E	503	9,1	14,14,15	0.86	0	15,19,21	1.02	1 (6%)
9	NAG	E	504	9	14,14,15	0.56	0	15,19,21	0.95	0
9	BMA	E	505	9	11,11,12	0.91	0	14,15,17	1.26	1 (7%)
9	MAN	E	506	9	11,11,12	0.58	0	14,15,17	1.03	1 (7%)
9	MAN	E	507	9	11,11,12	0.58	0	14,15,17	0.83	0
5	NAG	E	508	1,5	14,14,15	0.72	0	15,19,21	0.82	0
5	NAG	E	509	5	14,14,15	0.50	0	15,19,21	0.90	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	404	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	405	4	-	0/6/23/26	0/1/1/1
4	BMA	A	406	4	-	0/2/19/22	0/1/1/1
4	MAN	A	407	4	-	0/2/19/22	0/1/1/1
5	NAG	A	408	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	409	5	-	0/6/23/26	0/1/1/1
5	NAG	C	501	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	502	5	-	0/6/23/26	0/1/1/1
5	NAG	C	503	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	504	5	-	0/6/23/26	0/1/1/1
7	NAG	C	505	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	506	7	-	0/6/23/26	0/1/1/1
7	BMA	C	507	7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	508	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	509	5	-	0/6/23/26	0/1/1/1
5	NAG	D	201	2,5	-	0/6/23/26	0/1/1/1
5	NAG	D	202	5	-	0/6/23/26	0/1/1/1
9	NAG	E	503	9,1	-	0/6/23/26	0/1/1/1
9	NAG	E	504	9	-	0/6/23/26	0/1/1/1
9	BMA	E	505	9	-	0/2/19/22	0/1/1/1
9	MAN	E	506	9	-	0/2/19/22	0/1/1/1
9	MAN	E	507	9	-	0/2/19/22	0/1/1/1
5	NAG	E	508	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	509	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	505	NAG	C2-N2-C7	-3.18	118.95	123.04
5	D	202	NAG	C2-N2-C7	-2.98	119.21	123.04
4	A	404	NAG	C2-N2-C7	-2.70	119.57	123.04
7	C	505	NAG	C6-C5-C4	-2.59	106.62	113.02
9	E	506	MAN	O5-C1-C2	-2.55	106.72	110.86
7	C	505	NAG	C3-C2-N2	-2.16	105.38	110.56
5	C	502	NAG	C2-N2-C7	-2.11	120.33	123.04
5	C	508	NAG	O7-C7-C8	-2.08	118.25	122.06
5	C	501	NAG	O5-C5-C6	2.12	111.95	107.35
9	E	503	NAG	C1-O5-C5	2.30	115.17	112.25
5	C	503	NAG	O5-C5-C6	2.39	112.52	107.35
5	C	509	NAG	C1-O5-C5	2.53	115.45	112.25
5	A	409	NAG	C1-O5-C5	2.59	115.54	112.25
5	C	501	NAG	C1-O5-C5	2.65	115.61	112.25
5	E	509	NAG	C1-O5-C5	2.80	115.80	112.25
5	C	504	NAG	C1-O5-C5	2.80	115.81	112.25
4	A	406	BMA	C1-C2-C3	2.85	112.92	109.54
7	C	507	BMA	C1-C2-C3	3.08	113.19	109.54
9	E	505	BMA	C1-C2-C3	3.17	113.29	109.54
5	D	201	NAG	C1-O5-C5	4.18	117.55	112.25
5	C	502	NAG	C1-O5-C5	4.23	117.62	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	503	NAG	1	0
9	E	505	BMA	2	0
9	E	506	MAN	2	0

## 5.6 Ligand geometry [i](#)

15 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	14,14,15	0.49	0	15,19,21	1.69	2 (13%)
3	NAG	A	402	1	14,14,15	0.55	0	15,19,21	1.22	1 (6%)
3	NAG	A	403	1	14,14,15	0.51	0	15,19,21	1.72	5 (33%)
6	SO4	A	410	-	4,4,4	0.18	0	6,6,6	0.11	0
3	NAG	B	201	2	14,14,15	0.73	0	15,19,21	1.07	1 (6%)
6	SO4	B	202	-	4,4,4	0.16	0	6,6,6	0.44	0
8	GOL	C	510	-	5,5,5	0.22	0	5,5,5	0.39	0
6	SO4	D	203	-	4,4,4	0.23	0	6,6,6	0.37	0
6	SO4	D	204	-	4,4,4	0.17	0	6,6,6	0.24	0
3	NAG	E	501	1	14,14,15	0.46	0	15,19,21	1.64	3 (20%)
3	NAG	E	502	1	14,14,15	0.44	0	15,19,21	0.74	0
6	SO4	E	510	-	4,4,4	0.22	0	6,6,6	0.12	0
8	GOL	E	511	-	5,5,5	0.40	0	5,5,5	0.19	0
3	NAG	F	201	2	14,14,15	0.58	0	15,19,21	2.23	3 (20%)
6	SO4	F	202	-	4,4,4	0.18	0	6,6,6	0.17	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	401	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	402	1	-	0/6/23/26	0/1/1/1
3	NAG	A	403	1	-	0/6/23/26	0/1/1/1
6	SO4	A	410	-	-	0/0/0/0	0/0/0/0
3	NAG	B	201	2	-	0/6/23/26	0/1/1/1
6	SO4	B	202	-	-	0/0/0/0	0/0/0/0
8	GOL	C	510	-	-	0/4/4/4	0/0/0/0
6	SO4	D	203	-	-	0/0/0/0	0/0/0/0
6	SO4	D	204	-	-	0/0/0/0	0/0/0/0
3	NAG	E	501	1	-	0/6/23/26	0/1/1/1
3	NAG	E	502	1	-	0/6/23/26	0/1/1/1
6	SO4	E	510	-	-	0/0/0/0	0/0/0/0
8	GOL	E	511	-	-	0/4/4/4	0/0/0/0
3	NAG	F	201	2	-	0/6/23/26	0/1/1/1
6	SO4	F	202	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	501	NAG	C4-C3-C2	-3.61	105.62	111.23
3	A	403	NAG	C3-C4-C5	-3.37	104.32	110.20
3	F	201	NAG	C2-N2-C7	-3.13	119.01	123.04
3	F	201	NAG	C6-C5-C4	-2.90	105.87	113.02
3	A	402	NAG	C4-C3-C2	-2.68	107.06	111.23
3	E	501	NAG	C2-N2-C7	-2.56	119.75	123.04
3	A	403	NAG	C2-N2-C7	-2.13	120.30	123.04
3	A	401	NAG	C4-C3-C2	-2.03	108.08	111.23
3	A	403	NAG	O4-C4-C3	2.18	115.24	110.34
3	B	201	NAG	C1-O5-C5	2.73	115.71	112.25
3	A	403	NAG	O5-C5-C6	2.88	113.59	107.35
3	A	403	NAG	C1-O5-C5	3.39	116.56	112.25
3	E	501	NAG	C1-O5-C5	3.83	117.11	112.25
3	A	401	NAG	C1-O5-C5	5.68	119.46	112.25
3	F	201	NAG	C1-O5-C5	7.11	121.27	112.25

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
6	D	203	SO4	1	0
3	F	201	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	318/323 (98%)	-0.31	4 (1%) 79 82	12, 23, 41, 65	0
1	C	317/323 (98%)	-0.29	6 (1%) 70 73	12, 23, 41, 61	0
1	E	318/323 (98%)	-0.38	4 (1%) 79 82	12, 23, 39, 60	0
2	B	172/174 (98%)	-0.15	3 (1%) 73 76	10, 20, 40, 79	0
2	D	171/174 (98%)	-0.33	1 (0%) 90 91	10, 19, 39, 69	0
2	F	171/174 (98%)	-0.20	2 (1%) 81 83	10, 20, 42, 82	0
All	All	1467/1491 (98%)	-0.29	20 (1%) 78 80	10, 22, 41, 82	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	58	LYS	4.8
2	F	58	LYS	3.6
2	D	58	LYS	3.3
1	C	222	TRP	3.2
2	F	59	THR	3.1
2	B	172	GLN	3.1
1	C	173	ASN	2.9
1	C	160	THR	2.9
1	E	9	PRO	2.9
1	C	189	GLN	2.8
1	C	159	SER	2.8
1	C	9	PRO	2.6
2	B	59	THR	2.4
1	E	173	ASN	2.4
1	A	159	SER	2.4
1	A	173	ASN	2.2
1	E	277	CYS	2.2
1	A	129	GLY	2.1
1	E	222	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	276	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	A	408	14/15	0.93	0.13	6.50	25,36,41,51	0
5	NAG	C	508	14/15	0.94	0.17	3.68	25,31,39,49	0
5	NAG	C	501	14/15	0.84	0.20	3.30	29,37,47,49	0
5	NAG	E	508	14/15	0.95	0.18	2.99	23,33,41,47	0
5	NAG	C	503	14/15	0.89	0.22	2.50	39,49,53,60	0
9	NAG	E	503	14/15	0.96	0.11	2.09	23,34,41,42	0
4	NAG	A	405	14/15	0.93	0.20	1.72	33,43,55,59	0
4	NAG	A	404	14/15	0.97	0.18	1.44	27,37,52,53	0
9	NAG	E	504	14/15	0.94	0.14	1.03	30,36,46,49	0
7	NAG	C	505	14/15	0.94	0.13	0.45	27,39,50,53	0
7	NAG	C	506	14/15	0.92	0.14	0.38	41,50,63,65	0
5	NAG	C	504	14/15	0.73	0.32	-	57,72,77,79	0
7	BMA	C	507	11/12	0.82	0.23	-	70,75,76,76	0
4	MAN	A	407	11/12	0.60	0.45	-	83,85,88,89	0
5	NAG	D	201	14/15	0.83	0.28	-	40,57,62,65	0
5	NAG	C	502	14/15	0.77	0.30	-	54,62,69,69	0
5	NAG	E	509	14/15	0.81	0.30	-	57,63,70,73	0
9	MAN	E	506	11/12	0.69	0.39	-	76,80,84,86	0
4	BMA	A	406	11/12	0.82	0.34	-	66,72,75,79	0
9	BMA	E	505	11/12	0.83	0.29	-	55,63,70,75	0
5	NAG	A	409	14/15	0.73	0.29	-	57,66,73,74	0
5	NAG	D	202	14/15	0.73	0.48	-	74,79,85,86	0
5	NAG	C	509	14/15	0.81	0.31	-	59,65,73,73	0
9	MAN	E	507	11/12	0.79	0.40	-	81,85,88,89	0



## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	A	401	14/15	0.64	0.33	13.46	58,66,71,72	0
8	GOL	C	510	6/6	0.91	0.22	7.92	38,45,48,49	0
3	NAG	E	502	14/15	0.86	0.24	5.40	46,56,59,61	0
3	NAG	F	201	14/15	0.88	0.27	4.78	36,52,61,62	0
3	NAG	A	402	14/15	0.79	0.22	4.33	34,48,51,54	0
3	NAG	A	403	14/15	0.84	0.24	3.47	36,44,46,48	0
6	SO4	E	510	5/5	0.96	0.18	1.88	38,41,42,43	5
3	NAG	E	501	14/15	0.83	0.17	1.51	38,49,54,56	0
6	SO4	A	410	5/5	0.92	0.18	1.48	54,54,55,55	5
8	GOL	E	511	6/6	0.94	0.14	1.28	32,39,43,43	0
6	SO4	B	202	5/5	0.97	0.10	1.02	55,57,58,62	0
6	SO4	D	204	5/5	0.97	0.11	0.32	51,54,55,56	0
6	SO4	D	203	5/5	1.00	0.07	-0.84	17,18,19,20	5
6	SO4	F	202	5/5	0.98	0.08	-0.85	53,55,58,59	0
3	NAG	B	201	14/15	0.87	0.27	-	39,53,60,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.