



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:22 PM GMT

PDB ID : 4XKG  
Title : Crystal structure of hemagglutinin from Taiwan (2013) H6N1 influenza virus  
in complex with 6'-SLN  
Authors : Tzarum, N.; Zhu, X.; Wilson, I.A.  
Deposited on : 2015-01-11  
Resolution : 2.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (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

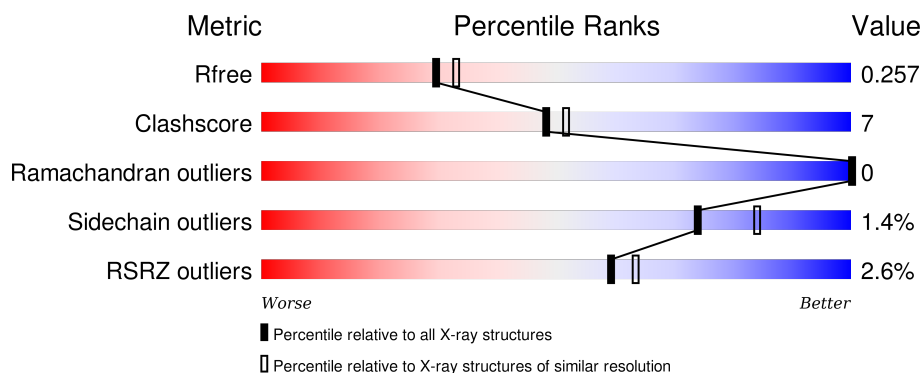
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 Å.

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




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	333	<div> <div>3%</div> <div>82%</div> <div>17%</div> <div>..</div> </div>
1	C	333	<div> <div>2%</div> <div>80%</div> <div>17%</div> <div>..</div> </div>
1	E	333	<div> <div>2%</div> <div>80%</div> <div>16%</div> <div>..</div> </div>
2	B	180	<div> <div>2%</div> <div>79%</div> <div>17%</div> <div>.</div> </div>
2	D	180	<div> <div>3%</div> <div>84%</div> <div>12%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	180	

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	402	-	-	-	X
3	NAG	D	201	-	-	-	X
3	NAG	F	201	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12441 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	330	Total	C	N	O	S	0	0	0
			2600	1648	443	496	13			
1	C	326	Total	C	N	O	S	0	0	0
			2569	1629	437	490	13			
1	E	325	Total	C	N	O	S	0	0	0
			2563	1626	437	487	13			

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

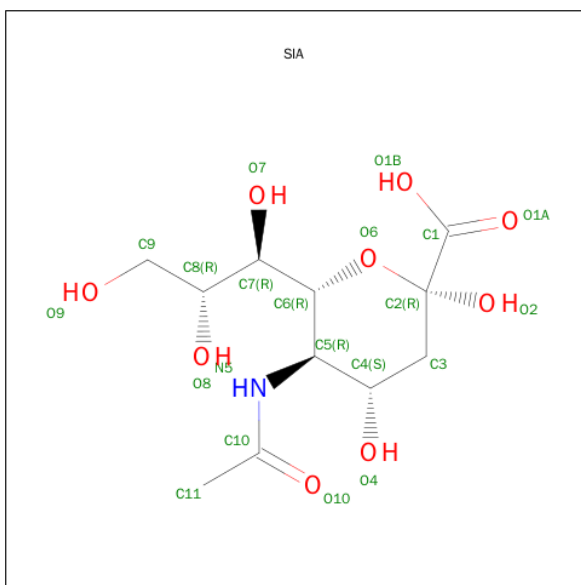
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1393	868	244	274	7			
2	D	173	Total	C	N	O	S	0	0	0
			1393	868	244	274	7			
2	F	172	Total	C	N	O	S	0	0	0
			1385	862	243	273	7			

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



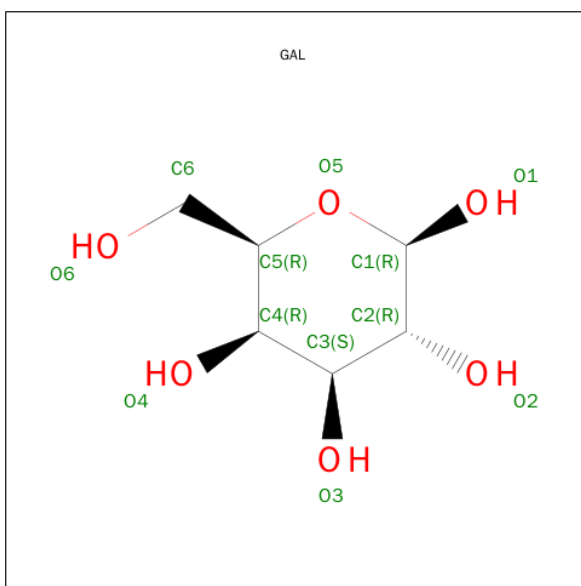
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is O-SIALIC ACID (three-letter code: SIA) (formula:  $C_{11}H_{19}NO_9$ ).



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

- Molecule 5 is BETA-D-GALACTOSE (three-letter code: GAL) (formula:  $C_6H_{12}O_6$ ).



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

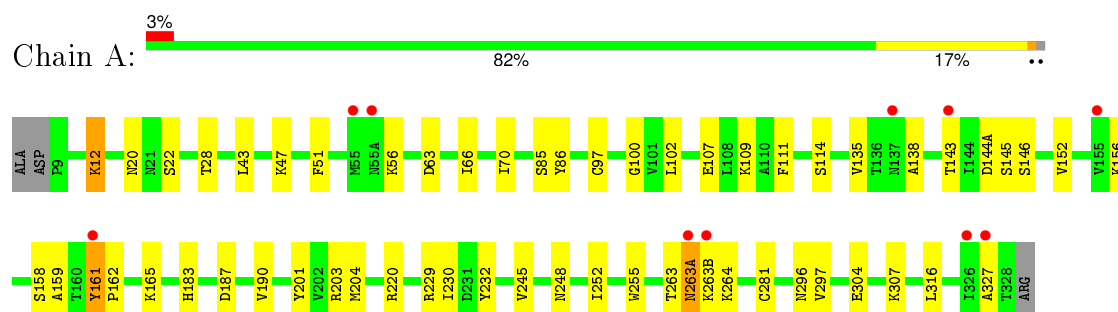
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	75	Total 75	O 75	0	0
6	B	52	Total 52	O 52	0	0
6	C	104	Total 104	O 104	0	0
6	D	42	Total 42	O 42	0	0
6	E	92	Total 92	O 92	0	0
6	F	57	Total 57	O 57	0	0

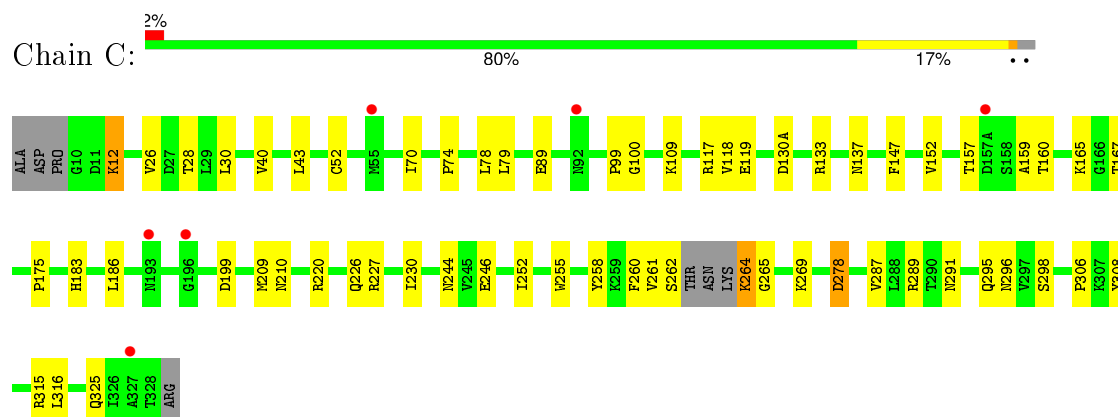
### 3 Residue-property plots [i](#)

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.

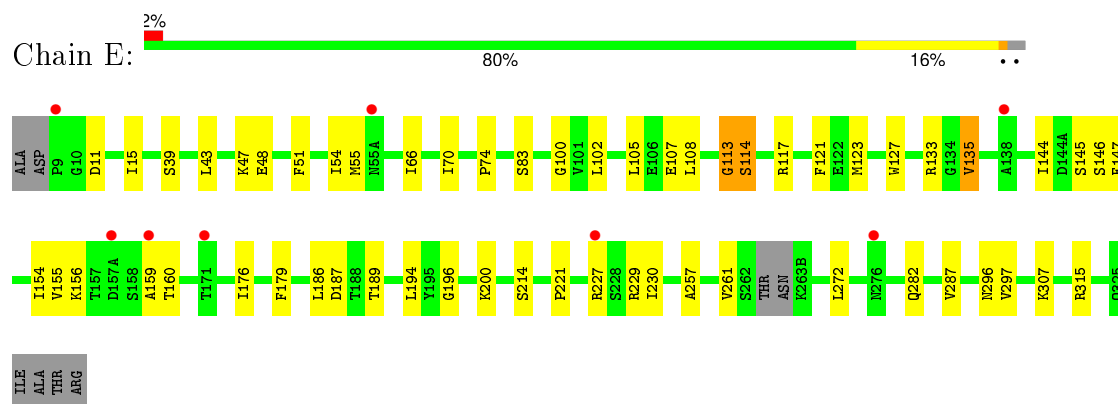
- Molecule 1: Hemagglutinin HA1 chain



- Molecule 1: Hemagglutinin HA1 chain

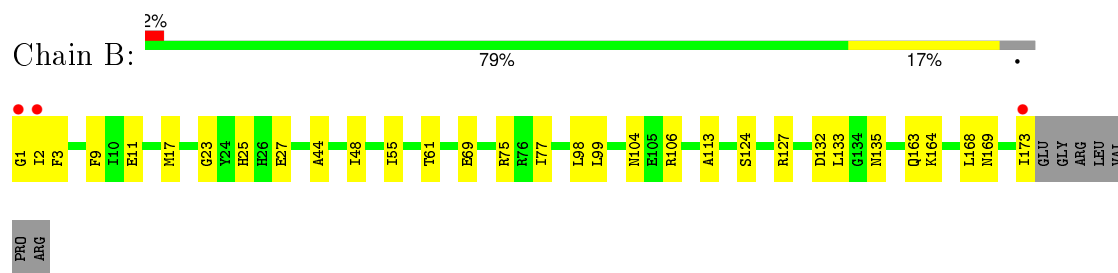


- Molecule 1: Hemagglutinin HA1 chain

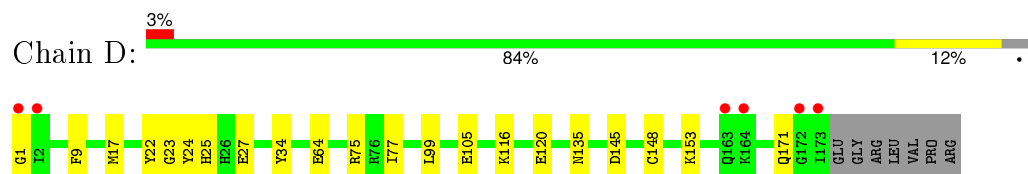




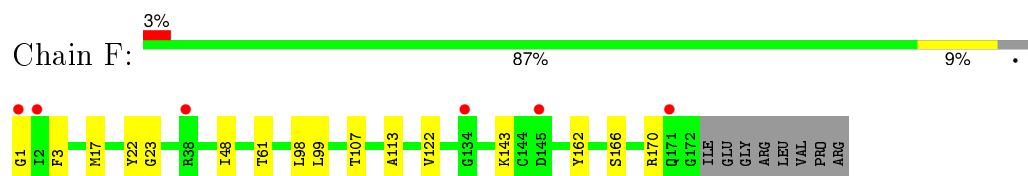
## ● Molecule 2: Hemagglutinin HA2 chain



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## ● Molecule 2: Hemagglutinin HA2 chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.46Å 99.06Å 133.67Å 90.00° 126.47° 90.00°	Depositor
Resolution (Å)	49.53 – 2.25 49.53 – 2.24	Depositor EDS
% Data completeness (in resolution range)	96.7 (49.53-2.25) 93.9 (49.53-2.24)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.90 (at 2.25Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.208 , 0.254 0.215 , 0.257	Depositor DCC
$R_{free}$ test set	4448 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.5	Xtriage
Anisotropy	0.825	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 57.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 90738 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12441	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: SIA, GAL, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.53	3/2662 (0.1%)	0.64	3/3622 (0.1%)
1	C	0.56	4/2629 (0.2%)	0.64	3/3576 (0.1%)
1	E	0.51	0/2624	0.62	1/3567 (0.0%)
2	B	0.52	0/1421	0.64	1/1913 (0.1%)
2	D	0.49	0/1421	0.61	1/1913 (0.1%)
2	F	0.48	0/1413	0.61	1/1902 (0.1%)
All	All	0.52	7/12170 (0.1%)	0.63	10/16493 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	109	LYS	CE-NZ	7.00	1.66	1.49
1	A	12	LYS	CD-CE	5.71	1.65	1.51
1	C	109	LYS	CD-CE	5.67	1.65	1.51
1	A	109	LYS	CE-NZ	5.62	1.63	1.49
1	C	12	LYS	CD-CE	5.49	1.65	1.51
1	C	12	LYS	CE-NZ	5.41	1.62	1.49
1	A	162	PRO	N-CD	5.35	1.55	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	LYS	CD-CE-NZ	9.44	133.42	111.70
2	B	1	GLY	N-CA-C	-8.13	92.76	113.10
1	C	12	LYS	CD-CE-NZ	7.84	129.73	111.70
1	C	265	GLY	N-CA-C	-6.85	95.96	113.10
1	A	161	TYR	C-N-CD	5.62	140.20	128.40
1	E	113	GLY	N-CA-C	-5.46	99.45	113.10
2	F	1	GLY	N-CA-C	-5.31	99.82	113.10
2	D	1	GLY	N-CA-C	-5.30	99.86	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	LEU	CA-CB-CG	5.08	126.99	115.30
1	C	316	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

There are no planarity outliers.

## 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	2600	0	2549	38	1
1	C	2569	0	2516	47	1
1	E	2563	0	2506	41	0
2	B	1393	0	1309	32	0
2	D	1393	0	1309	23	0
2	F	1385	0	1296	12	0
3	A	28	0	26	3	0
3	D	14	0	13	0	0
3	E	28	0	26	0	0
3	F	14	0	13	0	0
4	A	20	0	17	1	0
5	A	12	0	11	0	0
6	A	75	0	0	2	0
6	B	52	0	0	2	0
6	C	104	0	0	8	0
6	D	42	0	0	0	0
6	E	92	0	0	4	0
6	F	57	0	0	2	0
All	All	12441	0	11591	173	1

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 7.

All (173) 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)
2:B:77:ILE:CD1	2:D:77:ILE:HG22	1.71	1.20
2:B:77:ILE:HD11	2:D:77:ILE:CG2	1.80	1.10
2:B:77:ILE:CD1	2:D:77:ILE:CG2	2.32	1.08
2:B:77:ILE:HD11	2:D:77:ILE:HG22	0.93	0.93
1:A:114:SER:O	1:A:263:THR:HG22	1.74	0.88
2:B:17:MET:SD	2:B:23:GLY:HA3	2.19	0.82
1:A:263:THR:OG1	1:A:263(B):LYS:HG2	1.80	0.81
1:C:28:THR:HG22	1:C:30:LEU:H	1.46	0.78
2:F:162:TYR:OH	6:F:301:HOH:O	2.02	0.75
1:C:278:ASP:OD1	6:C:401:HOH:O	2.03	0.75
1:A:111:PHE:O	1:A:114:SER:HB2	1.88	0.74
1:A:263:THR:HG23	1:A:263(B):LYS:O	1.88	0.74
1:A:263(A):ASN:H	1:A:263(A):ASN:ND2	1.83	0.74
2:B:75:ARG:N	1:E:107:GLU:OE2	2.19	0.74
2:D:17:MET:SD	2:D:23:GLY:HA3	2.27	0.74
2:F:170:ARG:NH2	6:F:302:HOH:O	2.19	0.73
1:E:135:VAL:HG22	1:E:146:SER:HA	1.71	0.72
1:C:117:ARG:NH2	1:C:119:GLU:OE1	2.22	0.72
1:A:144(A):ASP:OD1	6:A:501:HOH:O	2.09	0.70
3:A:401:NAG:O3	3:A:401:NAG:H82	1.92	0.69
1:C:264:LYS:HE3	2:D:64:GLU:OE1	1.92	0.69
1:E:43:LEU:HD21	1:E:296:ASN:ND2	2.09	0.67
1:E:186:LEU:HD22	1:E:227:ARG:HB2	1.78	0.65
1:A:263(A):ASN:H	1:A:263(A):ASN:HD22	1.45	0.64
2:B:132:ASP:OD2	2:B:133:LEU:O	2.16	0.63
1:C:264:LYS:CE	2:D:64:GLU:OE1	2.48	0.62
2:B:98:LEU:HD21	2:F:99:LEU:HD13	1.81	0.62
1:C:183:HIS:HB2	1:C:252:ILE:HD11	1.83	0.60
1:A:97:CYS:HB2	1:A:138:ALA:O	2.02	0.60
1:C:40:VAL:HG13	1:C:40:VAL:O	2.01	0.59
1:C:28:THR:HG22	1:C:30:LEU:N	2.15	0.59
1:A:135:VAL:HG13	1:A:145:SER:HB3	1.85	0.59
1:E:102:LEU:HD23	1:E:105:LEU:CD1	2.33	0.58
1:C:12:LYS:NZ	2:D:25:HIS:NE2	2.44	0.58
1:C:298:SER:OG	6:C:402:HOH:O	2.17	0.58
1:A:187:ASP:HB3	1:A:190:VAL:H	1.68	0.58
2:B:163:GLN:NE2	2:D:171:GLN:HE22	2.02	0.57
1:E:15:ILE:HD11	2:F:122:VAL:HG21	1.85	0.57
1:C:165:LYS:HG2	1:C:246:GLU:HG3	1.85	0.57
1:E:307:LYS:NZ	2:F:61:THR:O	2.37	0.57
1:E:229:ARG:NE	6:E:509:HOH:O	2.37	0.57
1:E:135:VAL:HG13	1:E:145:SER:HB3	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:403:SIA:O7	4:A:403:SIA:O10	2.10	0.56
1:C:78:LEU:HD12	1:C:79:LEU:N	2.20	0.55
1:E:221:PRO:O	1:E:229:ARG:NH2	2.40	0.55
1:E:156:LYS:HB2	1:E:194:LEU:O	2.07	0.55
2:B:164:LYS:NZ	6:B:206:HOH:O	2.40	0.55
1:C:160:THR:O	6:C:404:HOH:O	2.18	0.55
2:B:77:ILE:CD1	2:D:77:ILE:HG21	2.35	0.54
1:C:262:SER:O	6:C:403:HOH:O	2.18	0.54
3:A:401:NAG:H82	3:A:401:NAG:C3	2.37	0.54
1:E:123:MET:HE2	1:E:257:ALA:HB2	1.88	0.54
2:D:145:ASP:HB3	2:D:148:CYS:H	1.72	0.54
1:E:11:ASP:OD2	2:F:143:LYS:HD2	2.07	0.54
1:E:54:ILE:HD11	1:E:282:GLN:HB2	1.90	0.54
1:A:43:LEU:HD21	1:A:296:ASN:ND2	2.23	0.53
1:C:152:VAL:HG23	1:C:255:TRP:HB2	1.91	0.53
2:B:69:GLU:OE1	6:B:201:HOH:O	2.19	0.53
1:C:325:GLN:HG2	6:C:430:HOH:O	2.08	0.53
1:E:66:ILE:O	1:E:70:ILE:HG13	2.07	0.53
1:C:159:ALA:HB1	1:C:160:THR:HA	1.92	0.52
1:C:52:CYS:SG	1:C:287:VAL:HG21	2.49	0.52
1:C:28:THR:HG23	2:D:105:GLU:HB2	1.91	0.52
1:A:56:LYS:HB3	1:A:85:SER:HB3	1.92	0.52
2:B:132:ASP:CG	2:B:133:LEU:O	2.48	0.52
1:A:28:THR:HG22	2:B:104:ASN:HB3	1.92	0.52
2:B:124:SER:HB2	2:B:127:ARG:NH2	2.24	0.52
1:A:107:GLU:OE2	2:D:75:ARG:N	2.34	0.51
1:E:47:LYS:HD3	1:E:297:VAL:HG13	1.93	0.51
1:A:152:VAL:HG23	1:A:255:TRP:HB2	1.92	0.51
2:D:17:MET:CE	2:D:23:GLY:HA3	2.40	0.51
1:A:135:VAL:HG22	1:A:146:SER:HA	1.93	0.50
2:D:116:LYS:HE3	2:D:120:GLU:OE2	2.11	0.50
1:C:78:LEU:CD1	1:C:79:LEU:CD2	2.89	0.50
1:A:135:VAL:CG1	1:A:145:SER:HB3	2.42	0.50
2:B:163:GLN:HE22	2:D:171:GLN:HE22	1.60	0.50
1:C:89:GLU:O	1:C:269:LYS:HA	2.12	0.50
1:E:102:LEU:HD21	1:E:108:LEU:CD2	2.42	0.50
1:C:295:GLN:HG2	1:C:306:PRO:HG2	1.94	0.49
1:E:135:VAL:HG22	1:E:146:SER:CA	2.40	0.49
1:E:102:LEU:HD23	1:E:105:LEU:HD12	1.95	0.49
1:C:78:LEU:HD12	1:C:79:LEU:HD23	1.95	0.49
1:A:281:CYS:HB2	1:A:304:GLU:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:LEU:HD13	1:C:227:ARG:HB2	1.95	0.48
1:C:99:PRO:HG3	1:C:226:GLN:HB2	1.95	0.48
1:C:220:ARG:NE	6:C:411:HOH:O	2.46	0.48
1:E:102:LEU:HD21	1:E:108:LEU:HD23	1.96	0.48
1:E:159:ALA:HB1	1:E:160:THR:HA	1.95	0.48
1:C:26:VAL:HG12	1:C:315:ARG:HG2	1.96	0.48
1:A:183:HIS:HB2	1:A:252:ILE:HD11	1.95	0.48
2:F:48:ILE:CD1	2:F:107:THR:HG23	2.44	0.47
1:C:175:PRO:HD2	1:C:260:PHE:O	2.14	0.47
1:E:187:ASP:HB3	1:E:189:THR:H	1.79	0.47
2:F:48:ILE:HD12	2:F:107:THR:HG23	1.96	0.47
1:E:196:GLY:H	1:E:200:LYS:HZ1	1.63	0.47
2:B:55:ILE:HG12	2:B:99:LEU:HD21	1.97	0.46
1:E:121:PHE:HZ	1:E:176:ILE:HD13	1.81	0.46
1:A:201:TYR:CD2	1:A:248:ASN:HB2	2.49	0.46
1:A:66:ILE:O	1:A:70:ILE:HG13	2.15	0.46
1:C:130(A):ASP:OD2	1:C:133:ARG:HD3	2.15	0.46
1:E:144:ILE:HD11	1:E:146:SER:HB2	1.97	0.46
1:C:291:ASN:OD1	1:C:291:ASN:N	2.49	0.46
1:C:12:LYS:HG2	2:D:27:GLU:HB3	1.98	0.46
1:E:100:GLY:HA3	1:E:230:ILE:O	2.16	0.46
1:C:78:LEU:CD1	1:C:79:LEU:HG	2.46	0.46
1:A:220:ARG:HB3	1:A:229:ARG:NH1	2.31	0.46
1:A:201:TYR:CD1	1:A:203:ARG:HG3	2.51	0.45
1:A:165:LYS:HA	1:A:245:VAL:O	2.16	0.45
1:E:113:GLY:O	1:E:114:SER:HB3	2.16	0.45
1:C:78:LEU:CD1	1:C:79:LEU:HD23	2.46	0.45
1:C:74:PRO:HG3	1:C:147:PHE:O	2.16	0.45
1:E:117:ARG:HB3	1:E:261:VAL:CG1	2.46	0.45
2:B:106:ARG:HH22	2:D:105:GLU:CD	2.18	0.45
1:C:117:ARG:HB3	1:C:261:VAL:HB	1.99	0.45
1:E:48:GLU:HB2	1:E:287:VAL:HB	1.98	0.45
1:A:47:LYS:HD3	1:A:297:VAL:HG13	1.99	0.45
2:D:17:MET:HE1	2:D:23:GLY:HA3	2.00	0.44
1:C:157:THR:HG22	6:C:404:HOH:O	2.17	0.44
1:E:70:ILE:HD13	1:E:179:PHE:CZ	2.52	0.44
1:A:12:LYS:HG2	2:B:27:GLU:HB3	2.00	0.44
1:E:39:SER:OG	1:E:315:ARG:HD3	2.17	0.44
1:A:263:THR:CG2	1:A:263(B):LYS:HG2	2.48	0.43
2:D:17:MET:HB2	2:D:34:TYR:HB3	1.99	0.43
2:B:2:ILE:HG23	2:B:3:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:17:MET:SD	2:F:23:GLY:HA3	2.58	0.43
1:A:201:TYR:CE2	1:A:248:ASN:HB2	2.53	0.43
1:A:203:ARG:O	1:A:204:MET:HG3	2.18	0.43
1:A:183:HIS:HB2	1:A:252:ILE:CD1	2.48	0.43
1:E:51:PHE:CE2	1:E:272:LEU:HB2	2.53	0.43
2:B:44:ALA:O	2:B:48:ILE:HG12	2.18	0.43
1:E:74:PRO:HG3	1:E:147:PHE:O	2.18	0.43
1:A:51:PHE:HB3	1:A:86:TYR:OH	2.19	0.43
2:B:124:SER:O	2:B:127:ARG:NE	2.44	0.43
1:E:229:ARG:NH2	6:E:509:HOH:O	2.52	0.42
1:A:12:LYS:HZ2	2:B:25:HIS:CD2	2.34	0.42
2:B:2:ILE:HG23	2:B:3:PHE:N	2.33	0.42
2:B:169:ASN:O	2:B:173:ILE:HG12	2.19	0.42
1:E:55:MET:SD	6:E:526:HOH:O	2.62	0.42
1:C:78:LEU:HD12	1:C:79:LEU:CD2	2.49	0.42
1:E:102:LEU:HD23	1:E:105:LEU:HD13	2.00	0.42
1:C:78:LEU:HD11	1:C:79:LEU:CD2	2.50	0.42
1:C:78:LEU:HD12	1:C:79:LEU:HG	2.01	0.42
2:D:9:PHE:O	2:D:135:ASN:HA	2.20	0.42
1:C:295:GLN:O	1:C:308:TYR:HA	2.19	0.42
1:E:127:TRP:CD1	1:E:154:ILE:HD11	2.54	0.42
2:F:166:SER:O	2:F:170:ARG:HB2	2.19	0.42
1:E:146:SER:OG	1:E:147:PHE:N	2.53	0.42
1:C:133:ARG:N	6:C:416:HOH:O	2.51	0.42
2:D:24:TYR:HB2	2:D:153:LYS:HE2	2.02	0.42
1:A:20:ASN:OD1	1:A:22:SER:HB3	2.20	0.42
2:B:11:GLU:HG3	2:B:135:ASN:OD1	2.20	0.41
1:A:156:LYS:HD2	1:A:159:ALA:O	2.19	0.41
1:E:113:GLY:O	1:E:114:SER:CB	2.68	0.41
1:C:167:THR:HG22	1:C:244:ASN:OD1	2.20	0.41
2:B:9:PHE:O	2:B:135:ASN:HA	2.20	0.41
1:A:102:LEU:HA	1:A:232:TYR:HB2	2.03	0.41
2:F:3:PHE:CE1	2:F:113:ALA:HB2	2.55	0.41
2:D:99:LEU:HD13	2:F:98:LEU:HD21	2.03	0.41
1:C:70:ILE:HD12	1:C:70:ILE:HA	1.96	0.41
1:A:63:ASP:OD2	6:A:502:HOH:O	2.22	0.41
2:B:2:ILE:HG12	2:B:2:ILE:O	2.21	0.41
1:C:118:VAL:HB	1:C:258:TYR:HB3	2.03	0.41
1:C:100:GLY:HA3	1:C:230:ILE:O	2.21	0.41
1:E:54:ILE:HA	1:E:54:ILE:HD13	1.86	0.41
1:E:196:GLY:H	1:E:200:LYS:NZ	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:PHE:CE2	2:B:113:ALA:HB2	2.56	0.41
1:C:43:LEU:HD21	1:C:296:ASN:ND2	2.36	0.41
1:C:210:ASN:ND2	6:E:504:HOH:O	2.53	0.40
1:A:307:LYS:HE3	2:B:61:THR:O	2.20	0.40
2:B:124:SER:HB2	2:B:127:ARG:HH21	1.86	0.40
1:A:100:GLY:HA3	1:A:230:ILE:O	2.21	0.40
3:A:402:NAG:C7	3:A:402:NAG:O3	2.70	0.40
2:B:168:LEU:HA	2:B:168:LEU:HD23	1.88	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ALA:O	1:C:137:ASN:OD1[3_555]	1.88	0.32

## 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	328/333 (98%)	318 (97%)	10 (3%)	0	100	100
1	C	322/333 (97%)	317 (98%)	5 (2%)	0	100	100
1	E	321/333 (96%)	303 (94%)	18 (6%)	0	100	100
2	B	171/180 (95%)	166 (97%)	5 (3%)	0	100	100
2	D	171/180 (95%)	167 (98%)	4 (2%)	0	100	100
2	F	170/180 (94%)	167 (98%)	3 (2%)	0	100	100
All	All	1483/1539 (96%)	1438 (97%)	45 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	289/291 (99%)	284 (98%)	5 (2%)	68	79
1	C	285/291 (98%)	280 (98%)	5 (2%)	66	77
1	E	284/291 (98%)	278 (98%)	6 (2%)	61	71
2	B	147/153 (96%)	147 (100%)	0	100	100
2	D	147/153 (96%)	146 (99%)	1 (1%)	88	93
2	F	146/153 (95%)	145 (99%)	1 (1%)	88	93
All	All	1298/1332 (97%)	1280 (99%)	18 (1%)	74	84

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	THR
1	A	158	SER
1	A	161	TYR
1	A	263(A)	ASN
1	A	264	LYS
1	C	199	ASP
1	C	209	MET
1	C	264	LYS
1	C	278	ASP
1	C	289	ARG
2	D	22	TYR
1	E	83	SER
1	E	114	SER
1	E	133	ARG
1	E	135	VAL
1	E	155	VAL
1	E	214	SER
2	F	22	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	263(A)	ASN
2	B	163	GLN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

8 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	0.50	0	15,19,21	0.73	0
3	NAG	A	402	1	14,14,15	0.83	1 (7%)	15,19,21	1.96	6 (40%)
4	SIA	A	403	-	16,20,21	0.77	0	18,28,31	1.42	3 (16%)
5	GAL	A	404	-	12,12,12	0.50	0	17,17,17	1.20	2 (11%)
3	NAG	D	201	2	14,14,15	0.67	0	15,19,21	1.44	3 (20%)
3	NAG	E	401	1	14,14,15	0.47	0	15,19,21	1.45	4 (26%)
3	NAG	E	402	1	14,14,15	0.47	0	15,19,21	1.06	2 (13%)
3	NAG	F	201	2	14,14,15	0.48	0	15,19,21	1.04	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
3	NAG	A	401	1	-	1/6/23/26	0/1/1/1
3	NAG	A	402	1	-	0/6/23/26	0/1/1/1
4	SIA	A	403	-	-	0/14/34/38	0/1/1/1
5	GAL	A	404	-	-	0/2/22/22	0/1/1/1
3	NAG	D	201	2	-	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	201	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	NAG	C2-N2	-2.02	1.42	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	NAG	C2-N2-C7	-4.21	117.63	123.04
5	A	404	GAL	O1-C1-C2	-3.32	100.31	109.21
3	A	402	NAG	C3-C2-N2	-3.28	102.70	110.56
3	A	402	NAG	O3-C3-C4	-2.97	103.65	110.34
3	E	401	NAG	C3-C2-N2	-2.89	103.64	110.56
3	D	201	NAG	O5-C5-C6	-2.31	102.35	107.35
3	A	402	NAG	C6-C5-C4	-2.03	108.01	113.02
3	A	402	NAG	O5-C5-C6	2.03	111.74	107.35
3	D	201	NAG	C2-N2-C7	2.03	125.65	123.04
3	E	401	NAG	C2-N2-C7	2.14	125.78	123.04
3	E	402	NAG	O5-C5-C6	2.20	112.11	107.35
3	E	401	NAG	O3-C3-C4	2.34	115.61	110.34
4	A	403	SIA	O6-C6-C5	2.42	112.45	108.48
4	A	403	SIA	O4-C4-C3	2.55	116.31	110.06
5	A	404	GAL	O1-C1-O5	2.61	117.38	110.25
3	D	201	NAG	C1-O5-C5	2.78	115.78	112.25
3	F	201	NAG	C1-O5-C5	2.89	115.92	112.25
3	A	402	NAG	C1-O5-C5	2.92	115.95	112.25
3	E	402	NAG	C1-O5-C5	2.92	115.96	112.25
4	A	403	SIA	C7-C6-C5	3.02	118.89	114.32
3	E	401	NAG	C1-O5-C5	3.02	116.08	112.25

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	NAG	2	0
3	A	402	NAG	1	0
4	A	403	SIA	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	330/333 (99%)	0.11	10 (3%) 54 58	27, 44, 60, 72	0
1	C	326/333 (97%)	0.03	6 (1%) 71 75	27, 38, 54, 74	0
1	E	325/333 (97%)	0.06	8 (2%) 61 65	28, 39, 53, 70	0
2	B	173/180 (96%)	0.23	3 (1%) 73 77	25, 35, 53, 72	0
2	D	173/180 (96%)	0.34	6 (3%) 48 52	26, 37, 56, 78	0
2	F	172/180 (95%)	0.20	6 (3%) 48 52	27, 37, 53, 78	0
All	All	1499/1539 (97%)	0.13	39 (2%) 59 63	25, 39, 56, 78	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1	GLY	6.2
2	B	1	GLY	5.7
2	F	1	GLY	5.3
1	A	55	MET	4.0
2	F	2	ILE	3.9
1	E	9	PRO	3.9
1	C	196	GLY	3.7
2	D	163	GLN	3.7
2	F	171	GLN	3.5
2	D	173	ILE	3.4
1	A	155	VAL	3.3
1	C	157(A)	ASP	3.2
2	B	173	ILE	3.2
1	C	92	ASN	3.1
1	C	327	ALA	3.0
1	A	263(B)	LYS	2.9
1	E	171	THR	2.9
1	A	327	ALA	2.7
1	E	55(A)	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	2	ILE	2.6
1	E	157(A)	ASP	2.5
2	D	164	LYS	2.5
1	A	55(A)	ASN	2.5
1	E	159	ALA	2.5
1	A	326	ILE	2.4
2	F	38	ARG	2.4
2	D	2	ILE	2.3
2	D	172	GLY	2.3
1	A	161	TYR	2.3
1	A	137	ASN	2.2
1	A	143	THR	2.1
2	F	145	ASP	2.1
1	C	55	MET	2.1
2	F	134	GLY	2.1
1	C	193	ASN	2.1
1	E	138	ALA	2.1
1	A	263(A)	ASN	2.0
1	E	227	ARG	2.0
1	E	276	ASN	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](#)

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(Å <sup>2</sup> )	Q<0.9
3	NAG	A	402	14/15	0.84	0.21	5.09	65,72,76,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	F	201	14/15	0.62	0.30	4.13	61,66,72,73	0
3	NAG	D	201	14/15	0.70	0.29	3.33	68,76,81,83	0
4	SIA	A	403	20/21	0.78	0.25	1.31	56,63,68,69	0
3	NAG	E	402	14/15	0.80	0.20	0.37	64,75,83,83	0
5	GAL	A	404	12/12	0.77	0.18	-	69,84,90,91	0
3	NAG	E	401	14/15	0.80	0.36	-	63,76,92,92	0
3	NAG	A	401	14/15	0.79	0.22	-	69,76,82,85	0

## 6.5 Other polymers

There are no such residues in this entry.