Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:04 PM GMT

PDB ID	:	3VUN
Title	:	Crystal structure of a influenza A virus (A/Aichi/2/1968 H3N2) hemagglutinin in C2 space group.
Authors	:	Yasutake, Y.; Suzuki, T.; Kawaguchi, A.; Nobusawa, E.
Deposited on	:	2012-07-02
Resolution	:	3.00 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

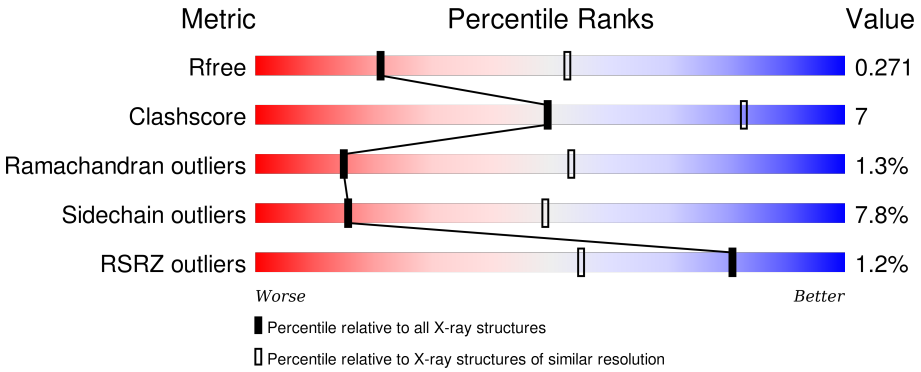
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 >=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 <=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	329	75% 18%
1	C	329	74% 19%
1	E	329	76% 18%
2	B	175	3% 81% 16%
2	D	175	2% 77% 19%

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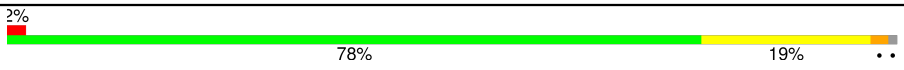
Mol	Chain	Length	Quality of chain
2	F	175	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12255 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2463	1540	432	478	13			
1	C	319	Total	C	N	O	S	0	0	0
			2463	1540	432	478	13			
1	E	319	Total	C	N	O	S	0	0	0
			2463	1540	432	478	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	144	SER	GLY	SEE REMARK 999	UNP P03437
A	182	VAL	ILE	SEE REMARK 999	UNP P03437
C	144	SER	GLY	SEE REMARK 999	UNP P03437
C	182	VAL	ILE	SEE REMARK 999	UNP P03437
E	144	SER	GLY	SEE REMARK 999	UNP P03437
E	182	VAL	ILE	SEE REMARK 999	UNP P03437

- 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
			1406	873	247	280	6			
2	D	173	Total	C	N	O	S	0	0	0
			1406	873	247	280	6			
2	F	173	Total	C	N	O	S	0	0	0
			1406	873	247	280	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	132	ASP	GLU	SEE REMARK 999	UNP P03437
D	132	ASP	GLU	SEE REMARK 999	UNP P03437

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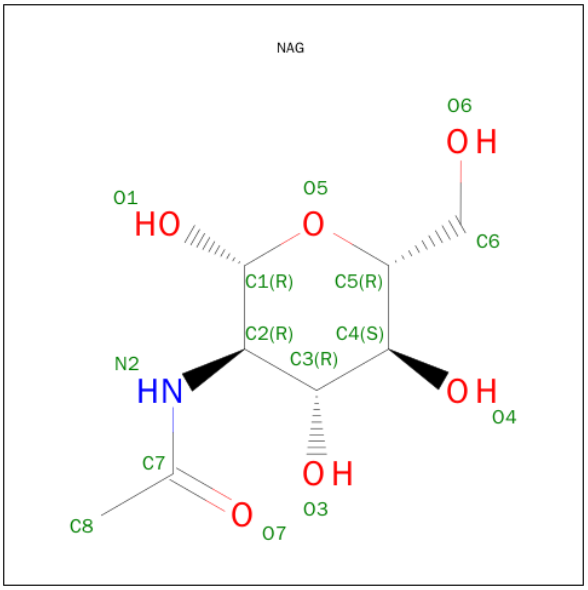
Chain	Residue	Modelled	Actual	Comment	Reference
F	132	ASP	GLU	SEE REMARK 999	UNP P03437

- 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	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	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	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is a polymer of unknown type called SUGAR (9-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	9	Total	C	N	O	0	0
			110	62	4	44		
4	C	9	Total	C	N	O	0	0
			110	62	4	44		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	9	Total	C	N	O	0	0
			110	62	4	44		

- 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	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

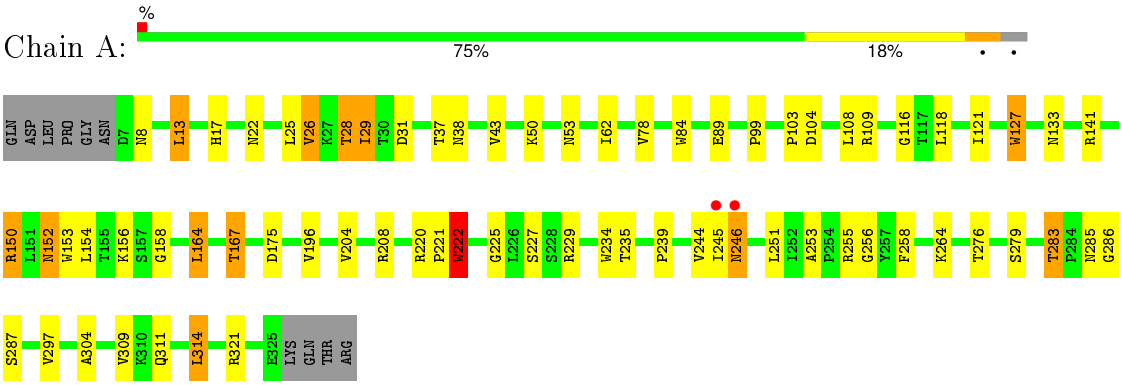
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	4	Total	C	N	O	0	0
			50	28	2	20		
6	C	4	Total	C	N	O	0	0
			50	28	2	20		
6	E	4	Total	C	N	O	0	0
			50	28	2	20		

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.

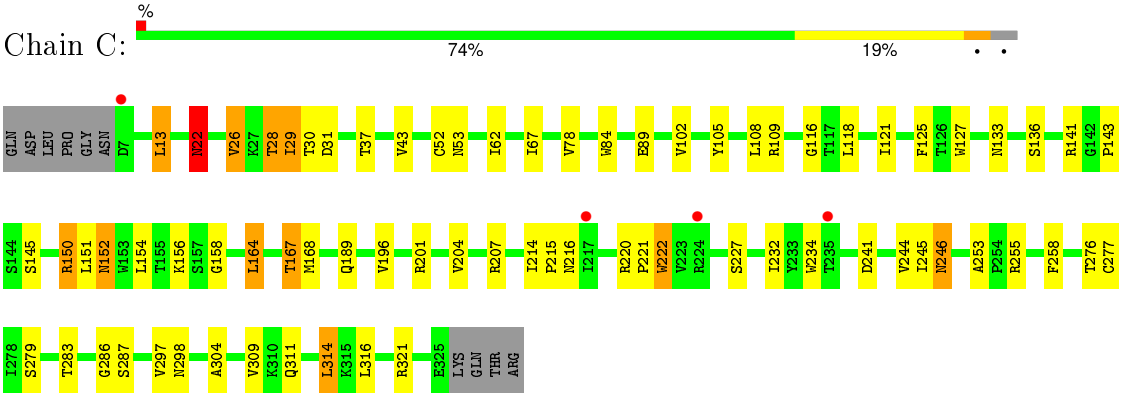
- Molecule 1: Hemagglutinin HA1 chain

Chain A:



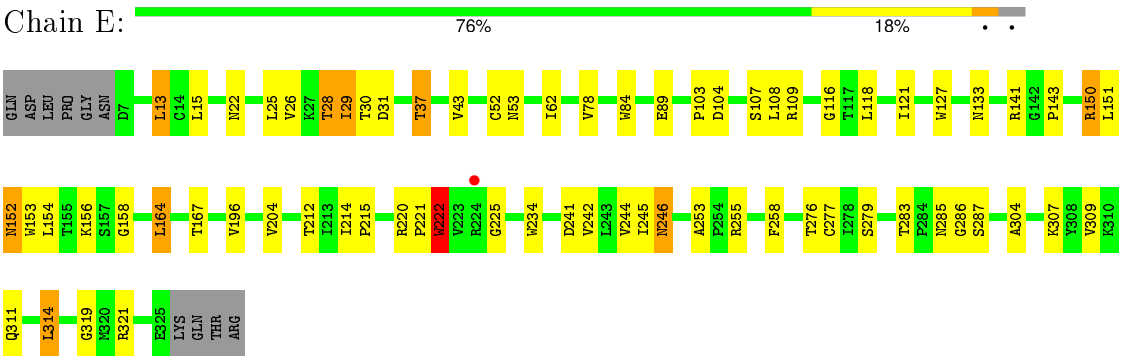
- Molecule 1: Hemagglutinin HA1 chain

Chain C:



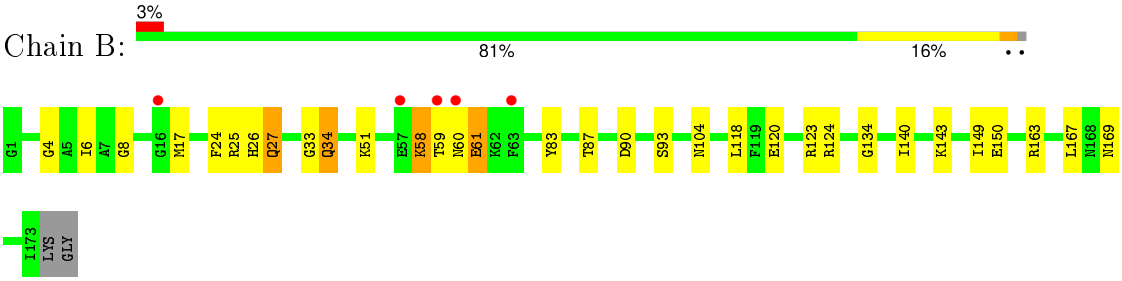
- Molecule 1: Hemagglutinin HA1 chain

Chain E:



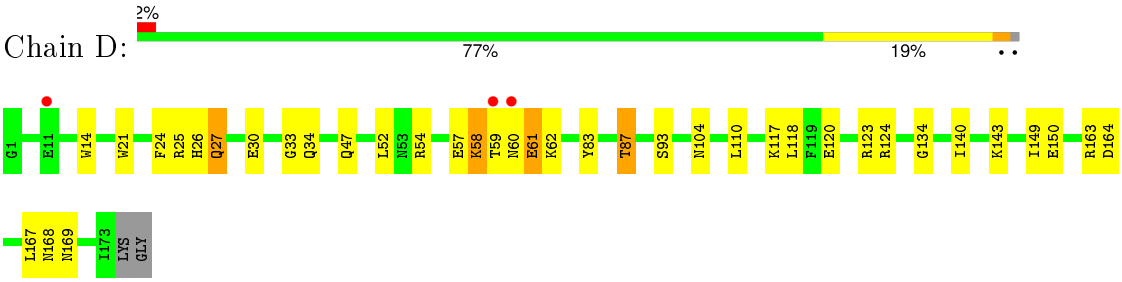
• Molecule 2: Hemagglutinin HA2 chain

Chain B:



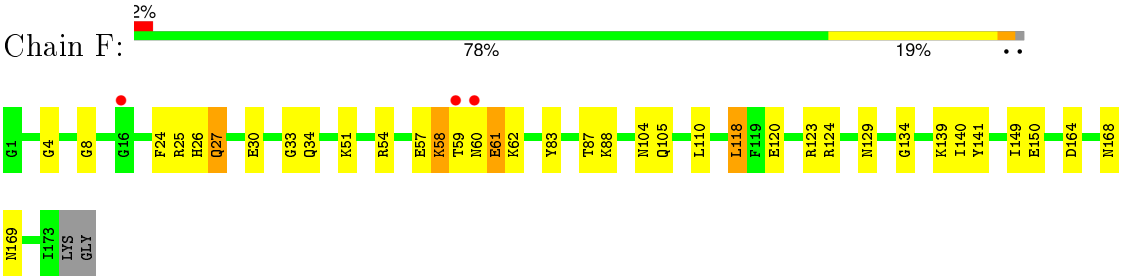
• Molecule 2: Hemagglutinin HA2 chain

Chain D:



• Molecule 2: Hemagglutinin HA2 chain

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	170.02Å 98.13Å 144.78Å 90.00° 113.11° 90.00°	Depositor
Resolution (Å)	30.59 – 3.00 30.59 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.59-3.00) 99.2 (30.59-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.95 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.216 , 0.275 0.213 , 0.271	Depositor DCC
R_{free} test set	2209 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	73.4	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 32.4	EDS
Estimated twinning fraction	0.457 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h +1/2*k-l 0.448 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h-1/2*k-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	0 of 43586 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12255	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: FUC, GAL, NAG, BMA, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.53	5/2519 (0.2%)	0.58	0/3434
1	C	0.48	2/2519 (0.1%)	0.58	0/3434
1	E	0.50	3/2519 (0.1%)	0.58	0/3434
2	B	0.48	0/1430	0.54	0/1922
2	D	0.48	2/1430 (0.1%)	0.54	0/1922
2	F	0.48	0/1430	0.54	0/1922
All	All	0.50	12/11847 (0.1%)	0.57	0/16068

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	TRP	CD2-CE2	9.31	1.52	1.41
1	A	153	TRP	CG-CD1	7.02	1.46	1.36
1	E	153	TRP	CD2-CE2	6.58	1.49	1.41
1	A	222	TRP	CD2-CE2	5.46	1.48	1.41
1	E	222	TRP	CD2-CE2	5.38	1.47	1.41
1	A	234	TRP	CD2-CE2	5.31	1.47	1.41
1	E	234	TRP	CD2-CE2	5.27	1.47	1.41
1	C	222	TRP	CD2-CE2	5.27	1.47	1.41
1	C	234	TRP	CD2-CE2	5.18	1.47	1.41
2	D	21	TRP	CD2-CE2	5.14	1.47	1.41
1	A	127	TRP	CD2-CE2	5.11	1.47	1.41
2	D	14	TRP	CD2-CE2	5.10	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2463	0	2403	39	0
1	C	2463	0	2403	46	0
1	E	2463	0	2403	44	0
2	B	1406	0	1327	18	0
2	D	1406	0	1327	21	0
2	F	1406	0	1327	21	0
3	A	14	0	13	2	0
3	B	14	0	13	0	0
3	C	14	0	13	1	0
3	D	14	0	13	0	0
3	E	14	0	13	1	0
3	F	14	0	13	0	0
4	A	110	0	94	2	0
4	C	110	0	94	1	0
4	E	110	0	94	3	0
5	A	28	0	25	1	0
5	C	28	0	25	0	0
5	E	28	0	25	1	0
6	A	50	0	43	0	0
6	C	50	0	43	0	0
6	E	50	0	43	0	0
All	All	12255	0	11754	171	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 7.

All (171) 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:283:THR:HG22	1:C:286:GLY:O	1.64	0.96
1:E:283:THR:HG22	1:E:286:GLY:O	1.67	0.95
1:A:283:THR:HG22	1:A:286:GLY:O	1.69	0.90
1:C:133:ASN:H	1:C:152:ASN:HD21	1.21	0.88
1:E:133:ASN:H	1:E:152:ASN:HD21	1.25	0.84
2:F:83:TYR:O	2:F:87:THR:HG23	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:304:ALA:HA	2:F:61:GLU:HB3	1.69	0.75
1:C:133:ASN:H	1:C:152:ASN:ND2	1.85	0.74
1:A:53:ASN:ND2	1:A:276:THR:HA	2.03	0.74
1:C:304:ALA:HA	2:D:61:GLU:HB3	1.71	0.72
1:E:89:GLU:OE2	1:E:109:ARG:NH2	2.21	0.72
2:F:120:GLU:OE1	2:F:123:ARG:NH2	2.23	0.72
1:E:133:ASN:H	1:E:152:ASN:ND2	1.88	0.71
1:A:133:ASN:H	1:A:152:ASN:HD21	1.38	0.71
1:C:89:GLU:OE2	1:C:109:ARG:NH2	2.22	0.71
1:A:89:GLU:OE2	1:A:109:ARG:NH2	2.24	0.71
2:D:83:TYR:O	2:D:87:THR:HG23	1.91	0.71
1:C:28:THR:HG22	1:C:31:ASP:H	1.54	0.71
2:B:26:HIS:CE1	2:B:33:GLY:HA3	2.27	0.69
2:D:26:HIS:CE1	2:D:33:GLY:HA3	2.27	0.69
2:D:120:GLU:OE1	2:D:123:ARG:NH2	2.26	0.68
1:A:28:THR:HG22	1:A:31:ASP:H	1.58	0.68
2:B:83:TYR:O	2:B:87:THR:HG23	1.93	0.68
2:F:26:HIS:CE1	2:F:33:GLY:HA3	2.30	0.67
1:E:28:THR:HG22	1:E:31:ASP:H	1.61	0.66
1:A:133:ASN:H	1:A:152:ASN:ND2	1.93	0.66
4:E:404:BMA:H61	4:E:405:MAN:H3	1.78	0.66
1:E:167:THR:HG22	1:E:244:VAL:HG22	1.76	0.65
4:A:404:BMA:H61	4:A:405:MAN:H3	1.78	0.65
1:E:53:ASN:ND2	1:E:276:THR:HA	2.11	0.65
1:A:28:THR:HG23	1:A:29:ILE:N	2.11	0.64
1:E:152:ASN:HB3	1:E:253:ALA:HB3	1.79	0.64
2:D:60:ASN:HD22	2:D:62:LYS:HE3	1.63	0.64
1:A:53:ASN:HD21	1:A:276:THR:HA	1.60	0.63
2:F:60:ASN:HD22	2:F:62:LYS:HE3	1.63	0.62
2:B:120:GLU:OE1	2:B:123:ARG:NH2	2.32	0.62
1:A:28:THR:HG23	1:A:29:ILE:H	1.64	0.62
1:C:28:THR:HG23	1:C:29:ILE:N	2.15	0.61
1:C:152:ASN:HB3	1:C:253:ALA:HB3	1.81	0.61
1:E:28:THR:HG22	1:E:31:ASP:N	2.16	0.60
1:E:13:LEU:HB2	2:F:140:ILE:HD11	1.84	0.60
1:E:309:VAL:HG13	1:E:311:GLN:OE1	2.03	0.58
1:A:28:THR:HG22	1:A:31:ASP:N	2.17	0.58
1:A:133:ASN:ND2	1:A:255:ARG:HH12	2.02	0.57
1:A:283:THR:HG23	1:A:285:ASN:H	1.70	0.57
1:C:28:THR:HG22	1:C:31:ASP:N	2.19	0.56
2:D:134:GLY:HA2	2:F:124:ARG:HD3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:THR:HG23	1:E:29:ILE:N	2.21	0.56
2:B:24:PHE:O	2:B:34:GLN:HA	2.06	0.56
1:A:121:ILE:HG23	4:A:403:NAG:H81	1.87	0.56
1:A:152:ASN:HB3	1:A:253:ALA:HB3	1.88	0.55
1:C:26:VAL:HG13	2:D:104:ASN:ND2	2.21	0.55
1:E:121:ILE:HG23	4:E:403:NAG:H81	1.86	0.55
1:C:283:THR:HG21	1:C:297:VAL:HG11	1.88	0.55
1:E:53:ASN:HD21	1:E:276:THR:HA	1.72	0.55
1:C:52:CYS:HB3	1:C:277:CYS:O	2.05	0.55
1:C:84:TRP:CE2	1:C:116:GLY:HA2	2.42	0.55
1:C:53:ASN:ND2	1:C:276:THR:HA	2.22	0.55
3:E:401:NAG:H3	3:E:401:NAG:H83	1.90	0.54
2:B:134:GLY:HA2	2:D:124:ARG:HD3	1.89	0.53
1:E:26:VAL:HG13	2:F:104:ASN:ND2	2.24	0.53
1:A:150:ARG:HG2	1:A:258:PHE:CZ	2.44	0.53
1:E:37:THR:HG22	1:E:319:GLY:HA3	1.91	0.53
1:E:283:THR:HG23	1:E:285:ASN:H	1.74	0.52
1:A:13:LEU:HB2	2:B:140:ILE:HD11	1.91	0.52
1:C:127:TRP:CZ2	1:C:253:ALA:HB1	2.44	0.52
3:C:401:NAG:H83	3:C:401:NAG:H3	1.91	0.51
1:C:150:ARG:HG2	1:C:258:PHE:CZ	2.45	0.51
1:A:28:THR:CG2	1:A:29:ILE:N	2.73	0.51
3:A:401:NAG:H83	3:A:401:NAG:H3	1.92	0.51
1:E:164:LEU:O	1:E:246:ASN:HA	2.11	0.51
1:A:127:TRP:CZ2	1:A:253:ALA:HB1	2.46	0.51
1:C:121:ILE:HG23	4:C:403:NAG:H81	1.91	0.50
1:A:309:VAL:HG13	1:A:311:GLN:OE1	2.11	0.50
1:E:167:THR:HG21	5:E:412:NAG:H82	1.93	0.50
1:E:204:VAL:HG22	1:E:245:ILE:HG12	1.93	0.50
2:D:26:HIS:ND1	2:D:149:ILE:HG21	2.26	0.50
1:E:43:VAL:HG23	1:E:314:LEU:HB2	1.93	0.50
1:A:84:TRP:CE2	1:A:116:GLY:HA2	2.48	0.49
1:E:150:ARG:HG2	1:E:258:PHE:CZ	2.47	0.49
1:E:133:ASN:ND2	1:E:255:ARG:HH12	2.11	0.49
1:C:125:PHE:HE1	1:C:168:MET:HB2	1.78	0.49
1:C:13:LEU:HB2	2:D:140:ILE:HD11	1.94	0.49
1:C:309:VAL:HG22	2:D:93:SER:HA	1.94	0.48
1:A:99:PRO:HB2	1:A:229:ARG:HD3	1.95	0.48
2:B:27:GLN:HE21	2:B:27:GLN:HA	1.77	0.48
2:B:163:ARG:O	2:B:167:LEU:HB2	2.14	0.48
2:D:27:GLN:HE21	2:D:27:GLN:HA	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:ARG:HB3	1:C:221:PRO:HD2	1.96	0.47
2:B:4:GLY:O	2:B:8:GLY:HA3	2.15	0.47
1:E:133:ASN:ND2	1:E:255:ARG:NH1	2.63	0.47
1:C:167:THR:HG23	1:C:244:VAL:HG22	1.97	0.47
1:E:151:LEU:O	1:E:255:ARG:NH2	2.48	0.47
1:C:150:ARG:HG2	1:C:258:PHE:HZ	1.80	0.47
1:C:22:ASN:N	1:C:22:ASN:OD1	2.46	0.47
2:D:24:PHE:O	2:D:34:GLN:HA	2.15	0.46
1:A:222:TRP:CD1	1:A:225:GLY:HA2	2.51	0.46
1:A:164:LEU:O	1:A:246:ASN:HA	2.15	0.46
1:E:103:PRO:O	1:E:104:ASP:OD1	2.34	0.46
1:A:167:THR:HG23	1:A:244:VAL:HG22	1.96	0.46
1:E:127:TRP:CZ2	1:E:253:ALA:HB1	2.50	0.46
1:A:279:SER:OG	1:A:287:SER:HB3	2.16	0.46
1:E:307:LYS:NZ	2:F:60:ASN:HD21	2.14	0.46
1:C:125:PHE:CE1	1:C:168:MET:HB2	2.50	0.46
1:C:207:ARG:HG2	1:C:241:ASP:OD1	2.16	0.46
2:D:47:GLN:OE1	2:D:110:LEU:HD11	2.16	0.45
5:A:411:NAG:H61	5:A:412:NAG:N2	2.30	0.45
2:F:139:LYS:HD2	2:F:141:TYR:CZ	2.52	0.45
2:D:54:ARG:O	2:D:57:GLU:HB2	2.16	0.45
2:F:4:GLY:O	2:F:8:GLY:HA3	2.15	0.45
1:E:84:TRP:CE2	1:E:116:GLY:HA2	2.51	0.45
2:F:24:PHE:O	2:F:34:GLN:HA	2.16	0.45
1:A:133:ASN:ND2	1:A:255:ARG:NH1	2.64	0.45
2:B:26:HIS:ND1	2:B:149:ILE:HG21	2.32	0.45
1:E:28:THR:HG23	2:F:105:GLN:OE1	2.17	0.45
2:F:27:GLN:HE21	2:F:27:GLN:HA	1.82	0.45
2:B:51:LYS:HB3	1:E:30:THR:HG22	1.98	0.45
2:B:4:GLY:CA	2:D:117:LYS:HE3	2.47	0.45
1:C:214:ILE:HA	1:C:215:PRO:HD3	1.85	0.45
1:C:283:THR:CG2	1:C:286:GLY:O	2.51	0.44
1:A:309:VAL:HG22	2:B:93:SER:HA	1.98	0.44
1:A:283:THR:HG21	1:A:297:VAL:HG11	2.00	0.44
1:A:220:ARG:HB3	1:A:221:PRO:HD2	1.98	0.44
1:E:214:ILE:HA	1:E:215:PRO:HD3	1.87	0.44
1:E:222:TRP:CD1	1:E:225:GLY:HA2	2.52	0.44
1:A:204:VAL:HG22	1:A:245:ILE:HG12	1.99	0.44
1:A:304:ALA:HA	2:B:61:GLU:HB3	1.99	0.44
1:E:220:ARG:HB3	1:E:221:PRO:HD2	1.98	0.44
1:A:150:ARG:HG2	1:A:258:PHE:HZ	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:ARG:HD3	2:F:134:GLY:HA2	2.00	0.44
1:E:150:ARG:HG2	1:E:258:PHE:HZ	1.83	0.43
1:E:279:SER:OG	1:E:287:SER:HB3	2.18	0.43
1:C:164:LEU:O	1:C:246:ASN:HA	2.18	0.43
1:A:43:VAL:HG23	1:A:314:LEU:HB2	1.99	0.43
1:E:52:CYS:HB3	1:E:277:CYS:O	2.18	0.43
1:A:103:PRO:O	1:A:104:ASP:OD1	2.36	0.43
2:F:26:HIS:ND1	2:F:149:ILE:HG21	2.32	0.43
1:C:151:LEU:O	1:C:255:ARG:NH2	2.50	0.43
1:A:38:ASN:ND2	3:A:401:NAG:C4	2.82	0.43
1:C:216:ASN:ND2	1:E:212:THR:HG21	2.34	0.43
1:C:28:THR:CG2	1:C:29:ILE:N	2.81	0.43
1:A:121:ILE:O	1:A:256:GLY:HA3	2.18	0.43
1:E:133:ASN:N	1:E:152:ASN:HD21	2.04	0.43
1:C:30:THR:HG22	2:F:51:LYS:HB3	2.00	0.43
1:C:279:SER:OG	1:C:287:SER:HB3	2.18	0.43
1:E:28:THR:CG2	1:E:29:ILE:N	2.81	0.43
1:C:316:LEU:HD23	2:D:52:LEU:HD12	2.01	0.43
1:C:53:ASN:HD21	1:C:276:THR:HA	1.84	0.42
2:F:164:ASP:O	2:F:168:ASN:HB2	2.19	0.42
1:C:102:VAL:HG22	1:C:232:ILE:HB	2.02	0.42
2:B:90:ASP:OD2	2:D:60:ASN:ND2	2.53	0.42
1:C:43:VAL:HG23	1:C:314:LEU:HB2	2.02	0.42
2:D:164:ASP:O	2:D:168:ASN:HB2	2.19	0.42
1:C:28:THR:HG23	1:C:29:ILE:H	1.81	0.42
1:E:241:ASP:OD1	1:E:242:VAL:N	2.50	0.42
1:A:175:ASP:OD1	1:A:239:PRO:HD3	2.20	0.42
4:E:404:BMA:H61	4:E:405:MAN:C3	2.46	0.41
1:C:136:SER:O	1:C:145:SER:HB2	2.20	0.41
2:D:163:ARG:O	2:D:167:LEU:HB2	2.19	0.41
1:A:17:HIS:CE1	2:B:6:ILE:HG23	2.54	0.41
1:C:283:THR:OG1	1:C:298:ASN:HB3	2.21	0.41
1:C:201:ARG:HE	1:C:201:ARG:HB3	1.74	0.41
1:C:28:THR:HG23	1:C:30:THR:H	1.86	0.41
1:C:204:VAL:HG22	1:C:245:ILE:HG12	2.02	0.41
1:C:67:ILE:HG13	1:C:105:TYR:CE1	2.56	0.41
1:C:309:VAL:HG13	1:C:311:GLN:OE1	2.21	0.41
2:F:54:ARG:O	2:F:57:GLU:HB2	2.21	0.40
2:D:87:THR:HG21	2:F:88:LYS:HD2	2.02	0.40
1:A:26:VAL:HG13	2:B:104:ASN:ND2	2.36	0.40
1:E:28:THR:CG2	1:E:30:THR:H	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:LEU:HD23	2:F:118:LEU:HD13	2.02	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	317/329 (96%)	293 (92%)	20 (6%)	4 (1%)	15	53
1	C	317/329 (96%)	291 (92%)	21 (7%)	5 (2%)	12	48
1	E	317/329 (96%)	295 (93%)	17 (5%)	5 (2%)	12	48
2	B	171/175 (98%)	156 (91%)	12 (7%)	3 (2%)	11	45
2	D	171/175 (98%)	158 (92%)	12 (7%)	1 (1%)	30	72
2	F	171/175 (98%)	157 (92%)	13 (8%)	1 (1%)	30	72
All	All	1464/1512 (97%)	1350 (92%)	95 (6%)	19 (1%)	15	53

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	22	ASN
1	C	62	ILE
1	A	22	ASN
1	E	22	ASN
1	E	158	GLY
1	A	62	ILE
1	A	196	VAL
2	B	34	GLN
2	D	58	LYS
1	E	62	ILE
1	E	143	PRO

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Mol	Chain	Res	Type
2	F	58	LYS
1	A	158	GLY
2	B	58	LYS
1	C	158	GLY
1	C	196	VAL
1	E	196	VAL
2	B	17	MET
1	C	143	PRO

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	282/291 (97%)	254 (90%)	28 (10%)	10	35
1	C	282/291 (97%)	260 (92%)	22 (8%)	16	49
1	E	282/291 (97%)	263 (93%)	19 (7%)	20	57
2	B	148/149 (99%)	138 (93%)	10 (7%)	20	56
2	D	148/149 (99%)	137 (93%)	11 (7%)	17	52
2	F	148/149 (99%)	137 (93%)	11 (7%)	17	52
All	All	1290/1320 (98%)	1189 (92%)	101 (8%)	16	49

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	13	LEU
1	A	25	LEU
1	A	26	VAL
1	A	28	THR
1	A	29	ILE
1	A	37	THR
1	A	50	LYS
1	A	78	VAL
1	A	108	LEU

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Mol	Chain	Res	Type
1	A	118	LEU
1	A	141	ARG
1	A	150	ARG
1	A	152	ASN
1	A	154	LEU
1	A	156	LYS
1	A	164	LEU
1	A	167	THR
1	A	208	ARG
1	A	222	TRP
1	A	227	SER
1	A	235	THR
1	A	246	ASN
1	A	251	LEU
1	A	264	LYS
1	A	283	THR
1	A	314	LEU
1	A	321	ARG
2	B	25	ARG
2	B	27	GLN
2	B	58	LYS
2	B	59	THR
2	B	60	ASN
2	B	61	GLU
2	B	118	LEU
2	B	143	LYS
2	B	150	GLU
2	B	169	ASN
1	C	13	LEU
1	C	22	ASN
1	C	26	VAL
1	C	28	THR
1	C	29	ILE
1	C	37	THR
1	C	78	VAL
1	C	108	LEU
1	C	118	LEU
1	C	141	ARG
1	C	150	ARG
1	C	152	ASN
1	C	154	LEU
1	C	156	LYS

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Mol	Chain	Res	Type
1	C	164	LEU
1	C	167	THR
1	C	189	GLN
1	C	222	TRP
1	C	227	SER
1	C	246	ASN
1	C	314	LEU
1	C	321	ARG
2	D	25	ARG
2	D	27	GLN
2	D	30	GLU
2	D	58	LYS
2	D	59	THR
2	D	61	GLU
2	D	87	THR
2	D	118	LEU
2	D	143	LYS
2	D	150	GLU
2	D	169	ASN
1	E	13	LEU
1	E	25	LEU
1	E	28	THR
1	E	29	ILE
1	E	37	THR
1	E	78	VAL
1	E	107	SER
1	E	108	LEU
1	E	118	LEU
1	E	141	ARG
1	E	150	ARG
1	E	152	ASN
1	E	154	LEU
1	E	156	LYS
1	E	164	LEU
1	E	222	TRP
1	E	246	ASN
1	E	314	LEU
1	E	321	ARG
2	F	25	ARG
2	F	27	GLN
2	F	30	GLU
2	F	58	LYS

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Mol	Chain	Res	Type
2	F	59	THR
2	F	61	GLU
2	F	110	LEU
2	F	118	LEU
2	F	129	ASN
2	F	150	GLU
2	F	169	ASN

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

Mol	Chain	Res	Type
1	A	8	ASN
1	A	53	ASN
1	A	96	ASN
1	A	132	GLN
1	A	133	ASN
1	A	152	ASN
1	A	171	ASN
1	A	216	ASN
2	B	27	GLN
2	B	49	ASN
2	B	125	GLN
2	B	169	ASN
1	C	96	ASN
1	C	132	GLN
1	C	152	ASN
1	C	171	ASN
1	C	216	ASN
2	D	27	GLN
2	D	60	ASN
1	E	96	ASN
1	E	132	GLN
1	E	133	ASN
1	E	152	ASN
1	E	171	ASN
1	E	296	ASN
2	F	27	GLN
2	F	60	ASN
2	F	125	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

45 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	402	1,4	14,14,15	0.75	0	15,19,21	1.08	1 (6%)
4	NAG	A	403	4	14,14,15	0.54	0	15,19,21	1.18	1 (6%)
4	BMA	A	404	4	11,11,12	0.39	0	14,15,17	1.79	1 (7%)
4	MAN	A	405	4	11,11,12	0.61	0	14,15,17	1.14	2 (14%)
4	NAG	A	406	4	14,14,15	0.50	0	15,19,21	1.11	1 (6%)
4	GAL	A	407	4	11,11,12	0.53	0	14,15,17	0.95	1 (7%)
4	FUC	A	408	4	10,10,11	1.34	1 (10%)	14,14,16	1.27	2 (14%)
4	MAN	A	409	4	11,11,12	0.48	0	14,15,17	1.44	1 (7%)
4	NAG	A	410	4	14,14,15	0.54	0	15,19,21	1.16	1 (6%)
5	NAG	A	411	1,5	14,14,15	0.59	0	15,19,21	0.97	2 (13%)
5	NAG	A	412	5	14,14,15	0.47	0	15,19,21	1.41	1 (6%)
6	NAG	A	413	1,6	14,14,15	0.50	0	15,19,21	1.25	1 (6%)
6	NAG	A	414	6	14,14,15	0.55	0	15,19,21	1.13	2 (13%)
6	BMA	A	415	6	11,11,12	0.54	0	14,15,17	0.83	0
6	MAN	A	416	6	11,11,12	0.56	0	14,15,17	1.51	2 (14%)
4	NAG	C	402	1,4	14,14,15	0.79	0	15,19,21	1.11	1 (6%)
4	NAG	C	403	4	14,14,15	0.51	0	15,19,21	1.11	1 (6%)
4	BMA	C	404	4	11,11,12	0.40	0	14,15,17	1.66	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	MAN	C	405	4	11,11,12	0.60	0	14,15,17	1.64	3 (21%)
4	NAG	C	406	4	14,14,15	0.54	0	15,19,21	1.08	1 (6%)
4	GAL	C	407	4	11,11,12	0.57	0	14,15,17	0.89	0
4	FUC	C	408	4	10,10,11	0.65	0	14,14,16	0.88	1 (7%)
4	MAN	C	409	4	11,11,12	0.52	0	14,15,17	1.31	1 (7%)
4	NAG	C	410	4	14,14,15	0.47	0	15,19,21	1.04	1 (6%)
5	NAG	C	411	1,5	14,14,15	0.62	0	15,19,21	1.10	2 (13%)
5	NAG	C	412	5	14,14,15	0.48	0	15,19,21	1.36	1 (6%)
6	NAG	C	413	1,6	14,14,15	0.49	0	15,19,21	1.29	3 (20%)
6	NAG	C	414	6	14,14,15	0.45	0	15,19,21	1.03	1 (6%)
6	BMA	C	415	6	11,11,12	0.51	0	14,15,17	0.94	0
6	MAN	C	416	6	11,11,12	0.63	0	14,15,17	1.98	3 (21%)
4	NAG	E	402	1,4	14,14,15	0.83	0	15,19,21	1.06	1 (6%)
4	NAG	E	403	4	14,14,15	0.46	0	15,19,21	1.02	1 (6%)
4	BMA	E	404	4	11,11,12	0.33	0	14,15,17	1.87	4 (28%)
4	MAN	E	405	4	11,11,12	0.58	0	14,15,17	1.25	2 (14%)
4	NAG	E	406	4	14,14,15	0.49	0	15,19,21	1.30	1 (6%)
4	GAL	E	407	4	11,11,12	0.57	0	14,15,17	0.89	1 (7%)
4	FUC	E	408	4	10,10,11	0.62	0	14,14,16	1.31	2 (14%)
4	MAN	E	409	4	11,11,12	0.52	0	14,15,17	1.33	1 (7%)
4	NAG	E	410	4	14,14,15	0.47	0	15,19,21	1.02	1 (6%)
5	NAG	E	411	1,5	14,14,15	0.66	0	15,19,21	1.36	2 (13%)
5	NAG	E	412	5	14,14,15	0.49	0	15,19,21	1.10	1 (6%)
6	NAG	E	413	1,6	14,14,15	0.50	0	15,19,21	1.28	1 (6%)
6	NAG	E	414	6	14,14,15	0.45	0	15,19,21	1.23	1 (6%)
6	BMA	E	415	6	11,11,12	0.47	0	14,15,17	0.70	0
6	MAN	E	416	6	11,11,12	0.60	0	14,15,17	1.65	2 (14%)

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	402	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	403	4	-	0/6/23/26	0/1/1/1
4	BMA	A	404	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	A	405	4	-	0/2/19/22	0/1/1/1
4	NAG	A	406	4	-	0/6/23/26	0/1/1/1
4	GAL	A	407	4	-	0/2/19/22	0/1/1/1
4	FUC	A	408	4	-	0/0/17/20	0/1/1/1
4	MAN	A	409	4	-	0/2/19/22	0/1/1/1
4	NAG	A	410	4	-	0/6/23/26	0/1/1/1
5	NAG	A	411	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	412	5	-	0/6/23/26	0/1/1/1
6	NAG	A	413	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	414	6	-	0/6/23/26	0/1/1/1
6	BMA	A	415	6	-	0/2/19/22	0/1/1/1
6	MAN	A	416	6	-	0/2/19/22	0/1/1/1
4	NAG	C	402	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	403	4	-	0/6/23/26	0/1/1/1
4	BMA	C	404	4	-	0/2/19/22	0/1/1/1
4	MAN	C	405	4	-	0/2/19/22	0/1/1/1
4	NAG	C	406	4	-	0/6/23/26	0/1/1/1
4	GAL	C	407	4	-	0/2/19/22	0/1/1/1
4	FUC	C	408	4	-	0/0/17/20	0/1/1/1
4	MAN	C	409	4	-	0/2/19/22	0/1/1/1
4	NAG	C	410	4	-	0/6/23/26	0/1/1/1
5	NAG	C	411	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	412	5	-	0/6/23/26	0/1/1/1
6	NAG	C	413	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	414	6	-	0/6/23/26	0/1/1/1
6	BMA	C	415	6	-	0/2/19/22	0/1/1/1
6	MAN	C	416	6	-	0/2/19/22	0/1/1/1
4	NAG	E	402	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	403	4	-	0/6/23/26	0/1/1/1
4	BMA	E	404	4	-	0/2/19/22	0/1/1/1
4	MAN	E	405	4	-	0/2/19/22	0/1/1/1
4	NAG	E	406	4	-	0/6/23/26	0/1/1/1
4	GAL	E	407	4	-	0/2/19/22	0/1/1/1
4	FUC	E	408	4	-	0/0/17/20	0/1/1/1
4	MAN	E	409	4	-	0/2/19/22	0/1/1/1
4	NAG	E	410	4	-	0/6/23/26	0/1/1/1
5	NAG	E	411	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	412	5	-	0/6/23/26	0/1/1/1
6	NAG	E	413	1,6	-	0/6/23/26	0/1/1/1
6	NAG	E	414	6	-	0/6/23/26	0/1/1/1
6	BMA	E	415	6	-	0/2/19/22	0/1/1/1
6	MAN	E	416	6	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	408	FUC	O5-C1	2.25	1.47	1.43

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	404	BMA	O3-C3-C4	-2.53	104.63	110.34
6	C	413	NAG	C3-C4-C5	-2.27	106.24	110.20
4	E	404	BMA	O3-C3-C4	-2.15	105.49	110.34
4	E	404	BMA	O3-C3-C2	-2.04	106.32	110.00
6	C	413	NAG	O4-C4-C5	2.01	114.58	109.24
4	C	408	FUC	C1-O5-C5	2.03	115.52	112.38
4	E	408	FUC	O5-C5-C6	2.07	109.55	106.13
5	A	411	NAG	C1-O5-C5	2.07	114.88	112.25
4	E	407	GAL	C1-O5-C5	2.08	114.88	112.25
5	C	411	NAG	C1-O5-C5	2.12	114.94	112.25
4	A	408	FUC	O5-C5-C4	2.17	113.29	109.53
6	A	414	NAG	C4-C3-C2	2.21	114.67	111.23
5	A	411	NAG	C4-C3-C2	2.25	114.72	111.23
6	C	413	NAG	C1-O5-C5	2.27	115.12	112.25
4	A	408	FUC	C1-O5-C5	2.27	115.88	112.38
4	E	403	NAG	C1-O5-C5	2.29	115.15	112.25
6	C	416	MAN	O5-C1-C2	2.31	114.61	110.86
6	A	414	NAG	C1-O5-C5	2.39	115.28	112.25
4	C	406	NAG	C1-O5-C5	2.46	115.37	112.25
4	E	405	MAN	C1-C2-C3	2.53	112.53	109.54
4	A	405	MAN	C1-C2-C3	2.59	112.60	109.54
4	A	405	MAN	C1-O5-C5	2.61	115.56	112.25
5	C	411	NAG	C4-C3-C2	2.68	115.40	111.23
4	A	406	NAG	C1-O5-C5	2.78	115.78	112.25
6	E	413	NAG	C1-O5-C5	2.79	115.79	112.25
4	C	410	NAG	C1-O5-C5	2.83	115.84	112.25
4	E	402	NAG	C4-C3-C2	2.85	115.67	111.23
4	C	403	NAG	C1-O5-C5	2.88	115.91	112.25
5	E	411	NAG	C1-O5-C5	2.94	115.98	112.25
4	A	407	GAL	C1-O5-C5	2.94	115.98	112.25
4	E	405	MAN	C1-O5-C5	2.95	116.00	112.25
5	E	412	NAG	C1-O5-C5	3.03	116.09	112.25
4	C	402	NAG	C4-C3-C2	3.04	115.95	111.23
4	C	405	MAN	O5-C1-C2	3.06	115.82	110.86
6	C	414	NAG	C1-O5-C5	3.11	116.20	112.25
4	C	404	BMA	C1-O5-C5	3.13	116.23	112.25
6	A	416	MAN	C1-C2-C3	3.14	113.26	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	402	NAG	C4-C3-C2	3.17	116.15	111.23
6	A	413	NAG	C1-O5-C5	3.23	116.35	112.25
4	E	404	BMA	C1-O5-C5	3.26	116.38	112.25
4	E	410	NAG	C1-O5-C5	3.27	116.40	112.25
4	A	403	NAG	C1-O5-C5	3.29	116.42	112.25
6	E	414	NAG	C1-O5-C5	3.31	116.44	112.25
4	C	405	MAN	C1-C2-C3	3.31	113.46	109.54
4	A	410	NAG	C1-O5-C5	3.31	116.45	112.25
4	C	405	MAN	C1-O5-C5	3.37	116.53	112.25
6	E	416	MAN	C1-C2-C3	3.49	113.66	109.54
5	E	411	NAG	C4-C3-C2	3.56	116.77	111.23
4	E	408	FUC	C1-O5-C5	3.58	117.90	112.38
4	E	409	MAN	C1-O5-C5	3.68	116.92	112.25
4	E	406	NAG	C1-O5-C5	3.68	116.92	112.25
4	C	404	BMA	C1-C2-C3	3.93	114.19	109.54
6	A	416	MAN	C1-O5-C5	4.00	117.33	112.25
4	C	409	MAN	C1-O5-C5	4.05	117.39	112.25
5	C	412	NAG	C1-O5-C5	4.37	117.79	112.25
6	E	416	MAN	C1-O5-C5	4.44	117.89	112.25
6	C	416	MAN	C1-C2-C3	4.44	114.80	109.54
5	A	412	NAG	C1-O5-C5	4.53	117.99	112.25
4	A	409	MAN	C1-O5-C5	4.62	118.11	112.25
4	E	404	BMA	C1-C2-C3	4.66	115.05	109.54
6	C	416	MAN	C1-O5-C5	4.81	118.36	112.25
4	A	404	BMA	C1-C2-C3	5.26	115.76	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	403	NAG	1	0
4	A	404	BMA	1	0
4	A	405	MAN	1	0
5	A	411	NAG	1	0
5	A	412	NAG	1	0
4	C	403	NAG	1	0
4	E	403	NAG	1	0
4	E	404	BMA	2	0
4	E	405	MAN	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	412	NAG	1	0

5.6 Ligand geometry (i)

6 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	0.73	0	15,19,21	2.77	5 (33%)
3	NAG	B	401	2	14,14,15	0.63	0	15,19,21	1.65	2 (13%)
3	NAG	C	401	1	14,14,15	0.71	0	15,19,21	2.81	5 (33%)
3	NAG	D	401	2	14,14,15	0.63	0	15,19,21	1.48	2 (13%)
3	NAG	E	401	1	14,14,15	0.71	0	15,19,21	2.67	5 (33%)
3	NAG	F	401	2	14,14,15	0.56	0	15,19,21	1.26	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	-	0/6/23/26	0/1/1/1
3	NAG	B	401	2	-	0/6/23/26	0/1/1/1
3	NAG	C	401	1	-	0/6/23/26	0/1/1/1
3	NAG	D	401	2	-	0/6/23/26	0/1/1/1
3	NAG	E	401	1	-	0/6/23/26	0/1/1/1
3	NAG	F	401	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	401	NAG	O7-C7-C8	-2.89	116.76	122.06
3	A	401	NAG	O7-C7-C8	-2.75	117.01	122.06
3	E	401	NAG	O7-C7-C8	-2.62	117.25	122.06
3	E	401	NAG	C3-C4-C5	2.23	114.09	110.20
3	A	401	NAG	C3-C4-C5	2.34	114.27	110.20
3	C	401	NAG	C3-C4-C5	2.67	114.85	110.20
3	D	401	NAG	C3-C4-C5	2.78	115.04	110.20
3	F	401	NAG	C4-C3-C2	3.10	116.05	111.23
3	E	401	NAG	C8-C7-N2	3.22	122.27	116.11
3	B	401	NAG	C3-C4-C5	3.26	115.88	110.20
3	A	401	NAG	C8-C7-N2	3.29	122.40	116.11
3	C	401	NAG	C8-C7-N2	3.41	122.63	116.11
3	E	401	NAG	C1-O5-C5	3.78	117.04	112.25
3	C	401	NAG	C1-O5-C5	3.94	117.25	112.25
3	A	401	NAG	C1-O5-C5	4.09	117.43	112.25
3	D	401	NAG	C4-C3-C2	4.20	117.75	111.23
3	B	401	NAG	C4-C3-C2	4.47	118.18	111.23
3	E	401	NAG	C2-N2-C7	7.75	133.00	123.04
3	A	401	NAG	C2-N2-C7	7.96	133.26	123.04
3	C	401	NAG	C2-N2-C7	8.11	133.46	123.04

There are no chirality outliers.

There are no torsion outliers.

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	C	401	NAG	1	0
3	E	401	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^{th} 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^2)	Q<0.9
1	A	319/329 (96%)	-0.01	2 (0%)	90	73	54, 79, 116, 139	0
1	C	319/329 (96%)	-0.00	4 (1%)	79	53	55, 79, 116, 151	0
1	E	319/329 (96%)	-0.01	1 (0%)	94	84	57, 79, 116, 142	0
2	B	173/175 (98%)	0.09	5 (2%)	55	26	53, 83, 114, 132	0
2	D	173/175 (98%)	0.01	3 (1%)	73	45	51, 85, 113, 136	0
2	F	173/175 (98%)	-0.01	3 (1%)	73	45	54, 84, 113, 136	0
All	All	1476/1512 (97%)	0.01	18 (1%)	81	55	51, 81, 115, 151	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	59	THR	4.6
2	B	60	ASN	4.5
2	B	59	THR	4.0
2	F	60	ASN	3.4
2	D	60	ASN	3.3
2	B	16	GLY	3.2
1	A	246	ASN	3.0
2	F	59	THR	3.0
1	C	224	ARG	2.9
1	E	224	ARG	2.8
1	C	7	ASP	2.8
2	D	11	GLU	2.6
1	A	245	ILE	2.6
2	F	16	GLY	2.5
1	C	217	ILE	2.4
2	B	63	PHE	2.3
1	C	235	THR	2.1
2	B	57	GLU	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^{th} 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^2)	Q<0.9
6	MAN	A	416	11/12	0.69	0.21	1.53	133,139,142,145	0
5	NAG	A	411	14/15	0.91	0.25	0.44	94,101,110,111	0
5	NAG	E	412	14/15	0.68	0.30	0.03	111,120,122,123	0
4	NAG	E	402	14/15	0.94	0.20	-0.11	63,65,73,76	0
4	FUC	E	408	10/11	0.95	0.22	-0.21	71,74,76,77	0
4	NAG	C	406	14/15	0.90	0.21	-0.31	84,100,104,107	0
5	NAG	E	411	14/15	0.93	0.19	-0.43	94,103,108,116	0
6	NAG	C	413	14/15	0.91	0.16	-0.43	73,82,92,104	0
4	NAG	E	406	14/15	0.84	0.21	-0.46	93,108,110,115	0
4	FUC	A	408	10/11	0.98	0.23	-0.49	71,74,75,81	0
4	FUC	C	408	10/11	0.97	0.18	-0.71	71,74,78,79	0
4	NAG	A	406	14/15	0.91	0.14	-0.95	94,107,111,116	0
5	NAG	C	411	14/15	0.96	0.19	-1.02	92,102,111,112	0
4	NAG	C	402	14/15	0.98	0.18	-1.22	60,64,71,74	0
4	NAG	A	402	14/15	0.96	0.15	-1.93	61,64,71,75	0
6	NAG	A	413	14/15	0.92	0.14	-1.94	75,81,93,106	0
5	NAG	C	412	14/15	0.88	0.15	-3.76	98,113,117,120	0
6	NAG	E	413	14/15	0.92	0.13	-4.27	78,86,97,107	0
5	NAG	A	412	14/15	0.88	0.18	-4.43	107,114,116,121	0
4	GAL	E	407	11/12	0.83	0.26	-	106,111,116,118	0
6	BMA	E	415	11/12	0.88	0.17	-	128,132,135,135	0
4	NAG	E	410	14/15	0.81	0.26	-	105,113,121,125	0
4	MAN	E	409	11/12	0.96	0.13	-	75,79,85,95	0
4	NAG	A	410	14/15	0.82	0.31	-	102,106,114,117	0
4	MAN	E	405	11/12	0.92	0.17	-	91,104,114,116	0
4	BMA	A	404	11/12	0.93	0.14	-	78,82,86,95	0
4	NAG	E	403	14/15	0.97	0.17	-	66,72,74,75	0
4	MAN	C	405	11/12	0.90	0.20	-	95,100,107,110	0
6	NAG	A	414	14/15	0.86	0.21	-	109,122,130,133	0
4	NAG	C	403	14/15	0.94	0.20	-	62,68,70,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	GAL	A	407	11/12	0.84	0.18	-	107,114,118,121	0
4	GAL	C	407	11/12	0.87	0.36	-	92,106,108,110	0
4	NAG	A	403	14/15	0.97	0.17	-	63,70,72,75	0
4	MAN	C	409	11/12	0.95	0.12	-	77,80,84,91	0
6	NAG	E	414	14/15	0.84	0.21	-	112,121,129,132	0
4	BMA	C	404	11/12	0.91	0.15	-	74,83,92,97	0
6	MAN	E	416	11/12	0.70	0.20	-	131,141,143,147	0
6	MAN	C	416	11/12	0.86	0.11	-	118,129,131,134	0
4	MAN	A	409	11/12	0.94	0.21	-	82,85,88,92	0
4	MAN	A	405	11/12	0.94	0.18	-	95,104,110,113	0
4	BMA	E	404	11/12	0.96	0.16	-	75,83,85,96	0
4	NAG	C	410	14/15	0.87	0.19	-	94,105,109,115	0
6	BMA	C	415	11/12	0.67	0.23	-	124,129,134,137	0
6	NAG	C	414	14/15	0.85	0.28	-	115,124,129,130	0
6	BMA	A	415	11/12	0.83	0.20	-	130,134,136,136	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^{th} 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^2)	Q<0.9
3	NAG	B	401	14/15	0.85	0.27	-	110,118,121,122	0
3	NAG	A	401	14/15	0.84	0.17	-	109,119,123,124	0
3	NAG	D	401	14/15	0.79	0.34	-	110,116,121,125	0
3	NAG	F	401	14/15	0.86	0.19	-	108,115,120,121	0
3	NAG	E	401	14/15	0.81	0.38	-	114,126,130,132	0
3	NAG	C	401	14/15	0.82	0.20	-	112,123,128,130	0

6.5 Other polymers (i)

There are no such residues in this entry.