Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:59 PM GMT

PDB ID	:	4K3X
Title	:	Crystal structure of a subtype H18 hemagglutinin homologue from A/flat-faced bat/Peru/033/2010 (H18N11)
Authors	:	Zhu, X.; Wilson, I.A.
Deposited on	:	2013-04-11
Resolution	:	2.15 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:

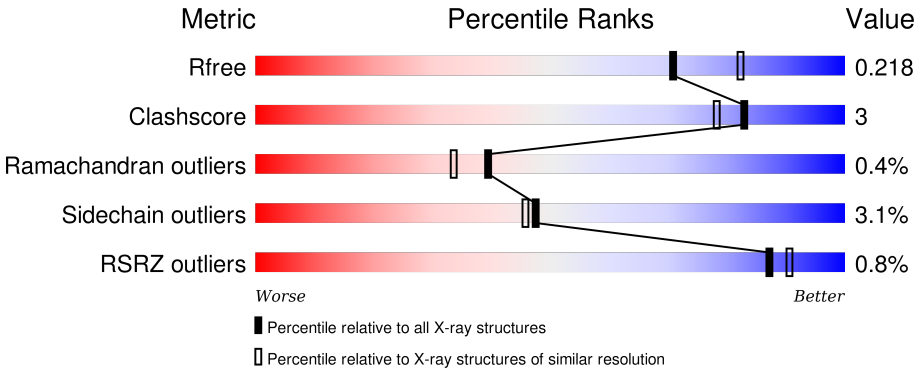
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.15 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	1693 (2.16-2.12)
Clashscore	102246	1824 (2.16-2.12)
Ramachandran outliers	100387	1798 (2.16-2.12)
Sidechain outliers	100360	1798 (2.16-2.12)
RSRZ outliers	91569	1699 (2.16-2.12)

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	2% 87% 9%
1	C	329	90% 7%
1	E	329	% 86% 10%
2	B	181	87% 6% 6%
2	D	181	% 87% 6% 6%

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Mol	Chain	Length	Quality of chain
2	F	181	86% 8% 6%

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	MAN	C	507	-	-	-	X
4	NAG	A	515	-	-	-	X
5	NAG	D	501	-	-	-	X
6	P4G	A	521	-	-	-	X
6	P4G	B	505	-	-	-	X
6	P4G	B	506	-	-	-	X
6	P4G	C	515	-	-	-	X
6	P4G	D	503	-	-	-	X
6	P4G	E	511	-	-	-	X
6	P4G	F	503	-	-	-	X
6	P4G	F	504	-	-	-	X
8	NAG	C	513	-	-	-	X
9	NAG	E	504	-	-	-	X
9	FUC	E	505	-	-	-	X
9	NAG	E	507	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 13212 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2533	1595	423	504	11			
1	C	322	Total	C	N	O	S	0	0	0
			2533	1595	423	504	11			
1	E	322	Total	C	N	O	S	0	0	0
			2533	1595	423	504	11			

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	170	Total	C	N	O	S	0	0	0
			1377	863	236	271	7			
2	D	170	Total	C	N	O	S	0	0	0
			1377	863	236	271	7			
2	F	170	Total	C	N	O	S	0	0	0
			1377	863	236	271	7			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	7	Total	C	N	O	0	0
			81	46	2	33		
3	A	7	Total	C	N	O	0	0
			81	46	2	33		
3	C	7	Total	C	N	O	0	0
			81	46	2	33		

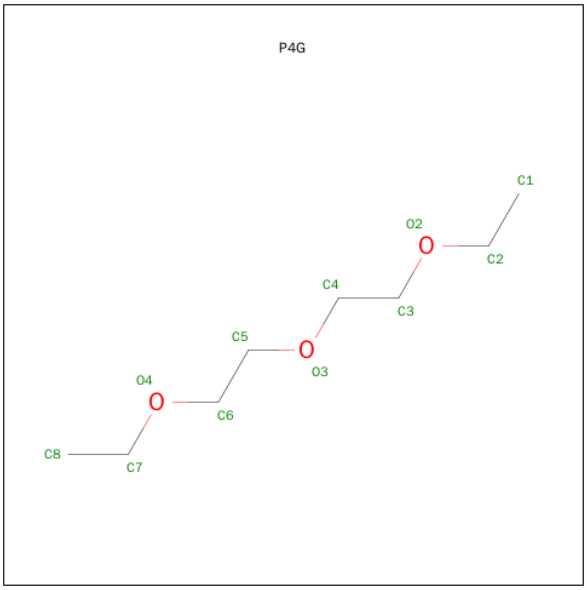
- Molecule 4 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	4	Total	C	N	O	0	0
			48	28	2	18		

- 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 28 16 2 10	0	0
5	E	2	Total C N O 28 16 2 10	0	0
5	E	2	Total C N O 28 16 2 10	0	0
5	D	2	Total C N O 28 16 2 10	0	0
5	F	2	Total C N O 28 16 2 10	0	0

- Molecule 6 is 1-ETHOXY-2-(2-ETHOXYETHOXY)ETHANE (three-letter code: P4G) (formula: $C_8H_{18}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 11 8 3	0	0
6	C	1	Total C O 11 8 3	0	0
6	C	1	Total C O 11 8 3	0	0
6	C	1	Total C O 11 8 3	0	0
6	E	1	Total C O 11 8 3	0	0

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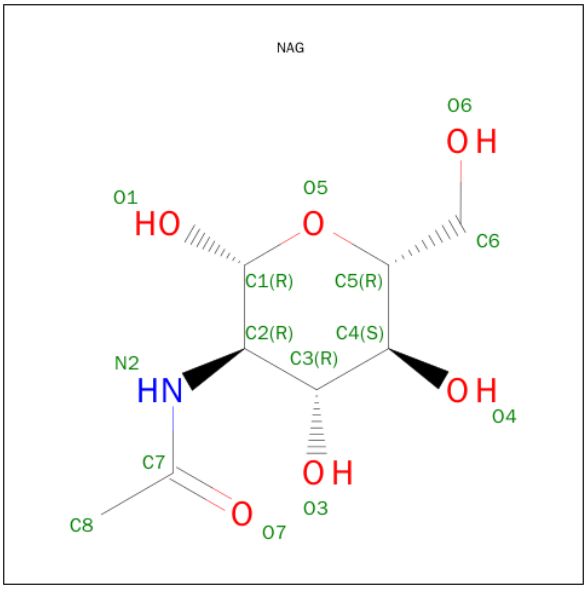
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total C O 11 8 3	0	0
6	B	1	Total C O 11 8 3	0	0
6	B	1	Total C O 11 8 3	0	0
6	B	1	Total C O 11 8 3	0	0
6	D	1	Total C O 11 8 3	0	0
6	F	1	Total C O 11 8 3	0	0
6	F	1	Total C O 11 8 3	0	0

- Molecule 7 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	5	Total C N O 60 34 2 24	0	0

- Molecule 8 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C N O 14 8 1 5	0	0

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	E	4	Total	C	N	O	0	0
			48	28	2	18		

- Molecule 10 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	3	Total	C	N	O	0	0
			38	22	2	14		

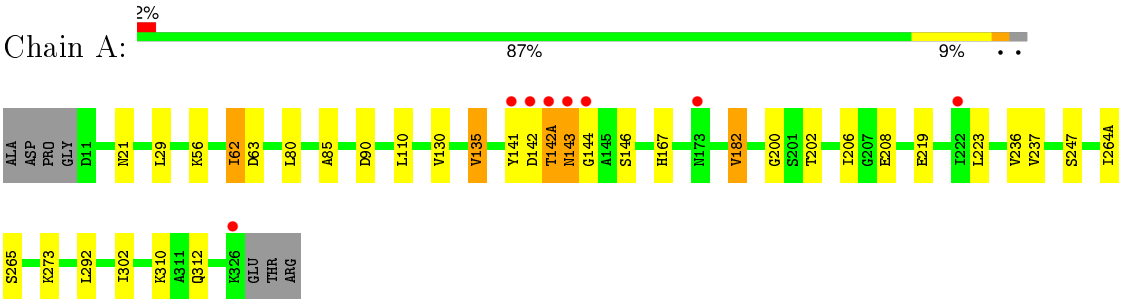
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	134	Total	O	0	0
			134	134		
11	C	201	Total	O	0	0
			201	201		
11	E	158	Total	O	0	0
			158	158		
11	B	89	Total	O	0	0
			89	89		
11	D	76	Total	O	0	0
			76	76		
11	F	87	Total	O	0	0
			87	87		

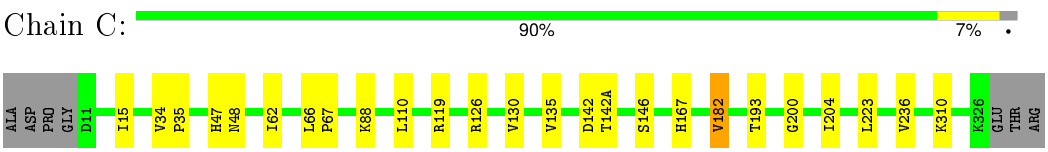
3 Residue-property plots (i)

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.

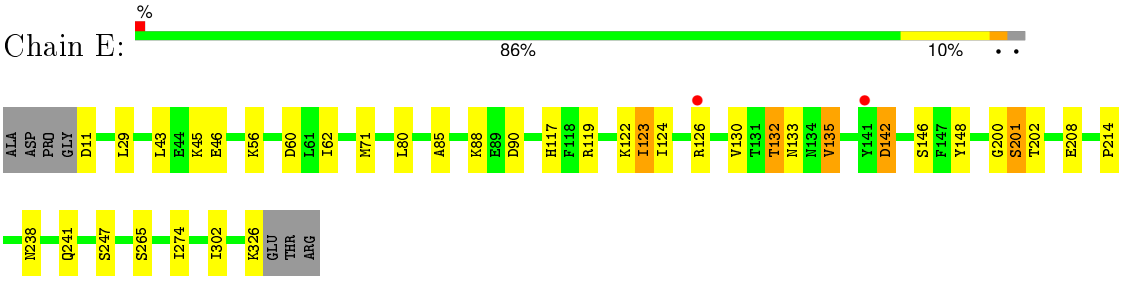
• Molecule 1: Hemagglutinin HA1



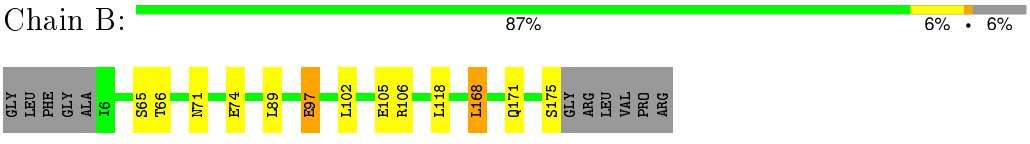
• Molecule 1: Hemagglutinin HA1



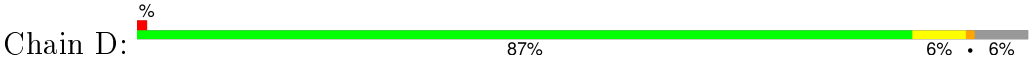
• Molecule 1: Hemagglutinin HA1

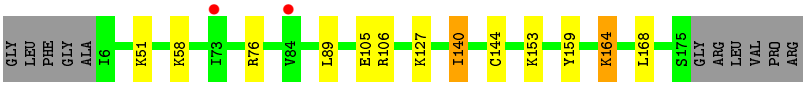


• Molecule 2: Hemagglutinin HA2



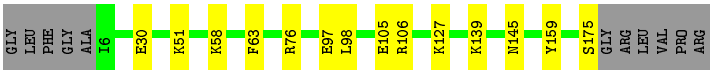
• Molecule 2: Hemagglutinin HA2





- Molecule 2: Hemagglutinin HA2

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	238.88Å 238.88Å 160.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.94 – 2.15 47.94 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.8 (47.94-2.15) 96.8 (47.94-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	3.78 (at 2.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.183 , 0.220 0.182 , 0.218	Depositor DCC
R_{free} test set	6095 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	36.8	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 121063 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13212	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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: BMA, NAG, P4G, FUC, FUL, 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	0.38	0/2591	0.53	0/3530
1	C	0.40	0/2591	0.54	0/3530
1	E	0.37	0/2591	0.51	0/3530
2	B	0.39	0/1403	0.48	0/1889
2	D	0.42	0/1403	0.50	0/1889
2	F	0.42	0/1403	0.50	0/1889
All	All	0.39	0/11982	0.51	0/16257

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	ASP	Peptide

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2533	0	2426	19	0
1	C	2533	0	2427	12	0
1	E	2533	0	2427	19	0
2	B	1377	0	1310	11	0
2	D	1377	0	1310	14	0
2	F	1377	0	1310	13	0
3	A	162	0	140	2	0
3	C	81	0	70	4	0
4	A	48	0	43	0	0
5	A	28	0	25	0	0
5	D	28	0	25	0	0
5	E	56	0	50	0	0
5	F	28	0	25	0	0
6	A	11	0	18	1	0
6	B	33	0	54	0	0
6	C	33	0	54	1	0
6	D	11	0	18	0	0
6	E	22	0	36	0	0
6	F	22	0	36	0	0
7	C	60	0	52	0	0
8	C	14	0	13	0	0
8	E	14	0	13	0	0
9	E	48	0	43	2	0
10	B	38	0	34	0	0
11	A	134	0	0	1	0
11	B	89	0	0	0	0
11	C	201	0	0	3	0
11	D	76	0	0	3	0
11	E	158	0	0	2	0
11	F	87	0	0	0	0
All	All	13212	0	11959	75	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 3.

All (75) 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:236:VAL:H	6:C:515:P4G:H71	1.50	0.75
2:B:105:GLU:CD	2:F:106:ARG:HH22	1.93	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:504:NAG:HO3	3:C:507:MAN:HO2	1.40	0.68
2:D:140:ILE:HD11	2:D:144:CYS:HB2	1.75	0.67
2:D:58:LYS:HD2	2:F:97:GLU:HG2	1.78	0.65
1:A:135:VAL:HG22	1:A:146:SER:HA	1.82	0.62
1:C:135:VAL:HG22	1:C:146:SER:HA	1.82	0.62
1:E:135:VAL:HG22	1:E:146:SER:HA	1.81	0.62
1:E:132:THR:HG23	1:E:133:ASN:OD1	2.00	0.61
1:E:122:LYS:NZ	11:E:694:HOH:O	2.26	0.61
1:C:48:ASN:N	11:C:747:HOH:O	2.33	0.61
2:D:153:LYS:NZ	11:D:653:HOH:O	2.35	0.60
9:E:504:NAG:H61	2:F:63:PHE:HB2	1.83	0.59
2:D:106:ARG:HH22	2:F:105:GLU:CD	2.07	0.58
1:A:310:LYS:HG3	2:B:89:LEU:HD11	1.86	0.58
2:D:164:LYS:NZ	2:F:175:SER:O	2.37	0.57
1:E:142:ASP:N	1:E:142:ASP:OD1	2.37	0.57
1:E:201:SER:HB2	1:E:214:PRO:HA	1.87	0.55
9:E:504:NAG:H5	9:E:505:FUC:H5	1.89	0.54
1:E:202:THR:HG23	1:E:247:SER:HB2	1.89	0.54
1:E:265:SER:HB2	1:E:302:ILE:HD13	1.90	0.53
2:F:127:LYS:HD3	2:F:159:TYR:CD1	2.45	0.52
2:B:102:LEU:O	2:B:106:ARG:HG3	2.10	0.52
3:C:504:NAG:O3	3:C:507:MAN:O2	2.17	0.52
2:B:106:ARG:HH22	2:D:105:GLU:CD	2.14	0.50
1:A:110:LEU:HD11	2:D:76:ARG:HA	1.93	0.50
1:A:236:VAL:H	6:A:521:P4G:H12	1.77	0.50
1:A:302:ILE:HD11	2:B:66:THR:HG22	1.94	0.50
2:B:105:GLU:OE2	2:F:106:ARG:NH2	2.44	0.50
2:F:30:GLU:OE1	2:F:145:ASN:HB2	2.13	0.49
1:A:29:LEU:HG	2:F:51:LYS:HG3	1.95	0.48
1:E:43:LEU:HD23	1:E:45:LYS:HD3	1.96	0.47
1:E:123:ILE:HG22	1:E:124:ILE:HG13	1.96	0.47
2:B:106:ARG:NH2	2:D:105:GLU:OE2	2.46	0.47
1:A:202:THR:HG23	1:A:247:SER:HB2	1.98	0.47
1:E:29:LEU:HG	2:D:51:LYS:HG3	1.97	0.46
2:B:97:GLU:HG2	2:F:58:LYS:HD2	1.96	0.46
3:A:512:BMA:H61	3:A:514:MAN:H2	1.42	0.46
1:C:310:LYS:HG3	2:D:89:LEU:HD11	1.98	0.46
1:E:238:ASN:O	1:E:241:GLN:HB2	2.15	0.46
1:E:71:MET:O	1:E:148:TYR:HB3	2.16	0.45
3:C:505:BMA:H61	3:C:507:MAN:H2	1.62	0.45
1:A:56:LYS:HB3	1:A:85:ALA:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:127:LYS:HD3	2:D:159:TYR:CD1	2.51	0.44
1:C:167:HIS:HB3	3:C:502:FUC:H62	1.99	0.44
1:A:62:ILE:HB	1:A:63:ASP:H	1.66	0.44
2:D:106:ARG:NE	11:D:661:HOH:O	2.40	0.43
1:C:182:VAL:HG22	11:C:605:HOH:O	2.18	0.43
1:C:47:HIS:HA	11:C:747:HOH:O	2.18	0.43
1:A:142(A):THR:HA	1:A:143:ASN:HA	1.69	0.43
2:D:106:ARG:NH2	11:D:661:HOH:O	2.47	0.42
2:F:98:LEU:HD23	2:F:98:LEU:HA	1.82	0.42
1:A:142(A):THR:HB	1:A:143:ASN:OD1	2.19	0.42
1:C:15:ILE:N	1:C:15:ILE:HD12	2.35	0.42
1:A:265:SER:HB2	1:A:302:ILE:HD13	2.01	0.41
1:A:206:ILE:HG23	1:A:237:VAL:HG22	2.01	0.41
1:C:66:LEU:HB3	1:C:67:PRO:HD3	2.02	0.41
2:B:168:LEU:O	2:B:171:GLN:HG2	2.20	0.41
1:E:80:LEU:CD2	11:E:720:HOH:O	2.68	0.41
1:A:167:HIS:HB3	3:A:502:FUC:H62	2.02	0.41
1:A:223:LEU:HD21	1:E:208:GLU:HB3	2.03	0.41
1:A:182:VAL:HG22	11:A:632:HOH:O	2.19	0.41
1:E:11:ASP:N	2:F:139:LYS:HZ2	2.19	0.41
1:A:141:TYR:CE2	1:A:146:SER:HB2	2.56	0.41
1:E:56:LYS:HB3	1:E:85:ALA:HB2	2.03	0.41
1:E:117:HIS:CE1	1:E:119:ARG:HE	2.39	0.41
1:E:43:LEU:HG	1:E:45:LYS:HG2	2.03	0.41
1:C:110:LEU:HD11	2:F:76:ARG:HA	2.03	0.41
2:D:127:LYS:HD3	2:D:159:TYR:CG	2.56	0.40
1:A:143:ASN:HB2	1:A:144:GLY:H	1.46	0.40
1:C:135:VAL:HG22	1:C:146:SER:CA	2.49	0.40
1:C:34:VAL:HA	1:C:35:PRO:HD3	1.94	0.40
1:E:60:ASP:HB2	1:E:274:ILE:HD13	2.03	0.40
1:A:264(A):ILE:O	2:B:65:SER:HB2	2.22	0.40
2:B:71:ASN:OD1	2:B:74:GLU:HG3	2.21	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	320/329 (97%)	311 (97%)	7 (2%)	2 (1%)	30 21
1	C	320/329 (97%)	313 (98%)	5 (2%)	2 (1%)	30 21
1	E	320/329 (97%)	313 (98%)	5 (2%)	2 (1%)	30 21
2	B	168/181 (93%)	165 (98%)	3 (2%)	0	100 100
2	D	168/181 (93%)	166 (99%)	2 (1%)	0	100 100
2	F	168/181 (93%)	167 (99%)	1 (1%)	0	100 100
All	All	1464/1530 (96%)	1435 (98%)	23 (2%)	6 (0%)	39 33

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ILE
1	A	200	GLY
1	C	62	ILE
1	C	200	GLY
1	E	62	ILE
1	E	200	GLY

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	290/295 (98%)	277 (96%)	13 (4%)	34 29
1	C	290/295 (98%)	280 (97%)	10 (3%)	44 41
1	E	290/295 (98%)	279 (96%)	11 (4%)	40 37
2	B	148/155 (96%)	144 (97%)	4 (3%)	52 52
2	D	148/155 (96%)	145 (98%)	3 (2%)	63 66
2	F	148/155 (96%)	148 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1314/1350 (97%)	1273 (97%)	41 (3%)	47 46

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	80	LEU
1	A	90	ASP
1	A	130	VAL
1	A	135	VAL
1	A	142(A)	THR
1	A	143	ASN
1	A	182	VAL
1	A	208	GLU
1	A	219	GLU
1	A	273	LYS
1	A	292	LEU
1	A	312	GLN
1	C	88	LYS
1	C	119	ARG
1	C	126	ARG
1	C	130	VAL
1	C	142	ASP
1	C	142(A)	THR
1	C	182	VAL
1	C	193	THR
1	C	204	ILE
1	C	223	LEU
1	E	46	GLU
1	E	88	LYS
1	E	90	ASP
1	E	123	ILE
1	E	126	ARG
1	E	130	VAL
1	E	132	THR
1	E	135	VAL
1	E	142	ASP
1	E	201	SER
1	E	326	LYS
2	B	97	GLU
2	B	118	LEU
2	B	168	LEU

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Mol	Chain	Res	Type
2	B	175	SER
2	D	140	ILE
2	D	164	LYS
2	D	168	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	289	ASN
2	B	95	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

47 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	$\#\|Z\|>2$
3	NAG	A	501	1,3	14,14,15	0.55	0	15,19,21	1.14	2 (13%)
3	FUC	A	502	3	10,10,11	0.57	0	14,14,16	1.02	2 (14%)
3	FUL	A	503	3	10,10,11	0.75	0	14,14,16	2.39	3 (21%)
3	NAG	A	504	3	14,14,15	0.52	0	15,19,21	0.92	1 (6%)
3	BMA	A	505	3	11,11,12	0.54	0	14,15,17	0.62	0
3	MAN	A	506	3	11,11,12	0.50	0	14,15,17	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	MAN	A	507	3	11,11,12	0.48	0	14,15,17	0.88	1 (7%)
3	NAG	A	508	1,3	14,14,15	0.61	0	15,19,21	0.93	1 (6%)
3	FUC	A	509	3	10,10,11	0.62	0	14,14,16	0.84	1 (7%)
3	FUL	A	510	3	10,10,11	0.63	0	14,14,16	1.36	3 (21%)
3	NAG	A	511	3	14,14,15	0.46	0	15,19,21	0.93	0
3	BMA	A	512	3	11,11,12	0.56	0	14,15,17	1.05	1 (7%)
3	MAN	A	513	3	11,11,12	0.52	0	14,15,17	0.84	0
3	MAN	A	514	3	11,11,12	0.52	0	14,15,17	0.80	1 (7%)
4	NAG	A	515	1,4	14,14,15	0.66	0	15,19,21	1.51	2 (13%)
4	FUL	A	516	4	10,10,11	0.59	0	14,14,16	1.13	1 (7%)
4	FUL	A	517	4	10,10,11	0.62	0	14,14,16	0.81	0
4	NAG	A	518	4	14,14,15	0.57	0	15,19,21	1.00	1 (6%)
5	NAG	A	519	1,5	14,14,15	0.55	0	15,19,21	0.66	0
5	NAG	A	520	5	14,14,15	0.48	0	15,19,21	0.78	1 (6%)
10	NAG	B	501	10,2	14,14,15	0.53	0	15,19,21	1.37	3 (20%)
10	FUL	B	502	10	10,10,11	0.55	0	14,14,16	0.94	1 (7%)
10	NAG	B	503	10	14,14,15	0.59	0	15,19,21	0.67	0
3	NAG	C	501	1,3	14,14,15	0.54	0	15,19,21	1.54	3 (20%)
3	FUC	C	502	3	10,10,11	0.62	0	14,14,16	1.00	2 (14%)
3	FUL	C	503	3	10,10,11	0.67	0	14,14,16	2.43	3 (21%)
3	NAG	C	504	3	14,14,15	0.57	0	15,19,21	0.97	2 (13%)
3	BMA	C	505	3	11,11,12	0.61	0	14,15,17	0.91	0
3	MAN	C	506	3	11,11,12	0.49	0	14,15,17	0.83	1 (7%)
3	MAN	C	507	3	11,11,12	0.48	0	14,15,17	0.92	0
7	NAG	C	508	1,7	14,14,15	0.56	0	15,19,21	0.80	1 (6%)
7	FUL	C	509	7	10,10,11	0.63	0	14,14,16	1.30	2 (14%)
7	NAG	C	510	7	14,14,15	0.54	0	15,19,21	1.73	3 (20%)
7	BMA	C	511	7	11,11,12	0.54	0	14,15,17	0.50	0
7	BMA	C	512	7	11,11,12	0.75	0	14,15,17	1.21	2 (14%)
5	NAG	D	501	2,5	14,14,15	0.53	0	15,19,21	1.01	1 (6%)
5	NAG	D	502	5	14,14,15	0.47	0	15,19,21	1.38	2 (13%)
5	NAG	E	501	1,5	14,14,15	0.46	0	15,19,21	0.85	1 (6%)
5	NAG	E	502	5	14,14,15	0.50	0	15,19,21	0.63	0
9	NAG	E	504	9,1	14,14,15	0.73	0	15,19,21	0.89	0
9	FUC	E	505	9	10,10,11	0.59	0	14,14,16	1.95	3 (21%)
9	FUL	E	506	9	10,10,11	0.59	0	14,14,16	0.71	1 (7%)
9	NAG	E	507	9	14,14,15	0.55	0	15,19,21	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	E	508	5	14,14,15	0.60	0	15,19,21	1.60	1 (6%)
5	NAG	E	509	5	14,14,15	0.49	0	15,19,21	0.64	0
5	NAG	F	501	2,5	14,14,15	0.60	0	15,19,21	0.72	0
5	NAG	F	502	5	14,14,15	0.54	0	15,19,21	0.80	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	501	1,3	-	0/6/23/26	0/1/1/1
3	FUC	A	502	3	-	0/0/17/20	0/1/1/1
3	FUL	A	503	3	-	0/0/17/20	0/1/1/1
3	NAG	A	504	3	-	0/6/23/26	0/1/1/1
3	BMA	A	505	3	-	0/2/19/22	0/1/1/1
3	MAN	A	506	3	-	0/2/19/22	0/1/1/1
3	MAN	A	507	3	-	0/2/19/22	0/1/1/1
3	NAG	A	508	1,3	-	0/6/23/26	0/1/1/1
3	FUC	A	509	3	-	0/0/17/20	0/1/1/1
3	FUL	A	510	3	-	0/0/17/20	0/1/1/1
3	NAG	A	511	3	-	0/6/23/26	0/1/1/1
3	BMA	A	512	3	-	0/2/19/22	0/1/1/1
3	MAN	A	513	3	-	0/2/19/22	0/1/1/1
3	MAN	A	514	3	-	0/2/19/22	0/1/1/1
4	NAG	A	515	1,4	-	0/6/23/26	0/1/1/1
4	FUL	A	516	4	-	0/0/17/20	0/1/1/1
4	FUL	A	517	4	-	0/0/17/20	0/1/1/1
4	NAG	A	518	4	-	0/6/23/26	0/1/1/1
5	NAG	A	519	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	520	5	-	0/6/23/26	0/1/1/1
10	NAG	B	501	10,2	-	0/6/23/26	0/1/1/1
10	FUL	B	502	10	-	0/0/17/20	0/1/1/1
10	NAG	B	503	10	-	0/6/23/26	0/1/1/1
3	NAG	C	501	1,3	-	0/6/23/26	0/1/1/1
3	FUC	C	502	3	-	0/0/17/20	0/1/1/1
3	FUL	C	503	3	-	0/0/17/20	0/1/1/1
3	NAG	C	504	3	-	0/6/23/26	0/1/1/1
3	BMA	C	505	3	-	0/2/19/22	0/1/1/1
3	MAN	C	506	3	-	0/2/19/22	0/1/1/1
3	MAN	C	507	3	-	0/2/19/22	1/1/1/1
7	NAG	C	508	1,7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FUL	C	509	7	-	0/0/17/20	0/1/1/1
7	NAG	C	510	7	-	0/6/23/26	0/1/1/1
7	BMA	C	511	7	-	0/2/19/22	0/1/1/1
7	BMA	C	512	7	-	0/2/19/22	0/1/1/1
5	NAG	D	501	2,5	-	0/6/23/26	0/1/1/1
5	NAG	D	502	5	-	0/6/23/26	0/1/1/1
5	NAG	E	501	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	502	5	-	0/6/23/26	0/1/1/1
9	NAG	E	504	9,1	-	0/6/23/26	0/1/1/1
9	FUC	E	505	9	-	0/0/17/20	0/1/1/1
9	FUL	E	506	9	-	0/0/17/20	0/1/1/1
9	NAG	E	507	9	-	0/6/23/26	0/1/1/1
5	NAG	E	508	5	-	0/6/23/26	0/1/1/1
5	NAG	E	509	5	-	0/6/23/26	0/1/1/1
5	NAG	F	501	2,5	-	0/6/23/26	0/1/1/1
5	NAG	F	502	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	503	FUL	C1-C2-C3	-6.09	102.34	109.54
3	A	503	FUL	C1-O5-C5	-5.75	103.49	112.38
3	A	503	FUL	C1-C2-C3	-5.72	102.77	109.54
3	C	503	FUL	C1-O5-C5	-5.55	103.80	112.38
4	A	515	NAG	C2-N2-C7	-4.09	117.78	123.04
3	C	501	NAG	C2-N2-C7	-4.03	117.87	123.04
3	A	501	NAG	O3-C3-C2	-3.42	102.33	109.11
3	A	510	FUL	C1-C2-C3	-3.06	105.92	109.54
4	A	518	NAG	C2-N2-C7	-3.02	119.15	123.04
7	C	509	FUL	C1-C2-C3	-2.99	106.00	109.54
3	A	504	NAG	C2-N2-C7	-2.61	119.69	123.04
5	D	501	NAG	C2-N2-C7	-2.59	119.71	123.04
3	C	502	FUC	O5-C1-C2	-2.52	106.76	110.86
3	A	507	MAN	O5-C1-C2	-2.50	106.80	110.86
5	A	520	NAG	C2-N2-C7	-2.36	120.00	123.04
3	A	502	FUC	O5-C1-C2	-2.35	107.04	110.86
3	A	510	FUL	C1-O5-C5	-2.34	108.77	112.38
7	C	512	BMA	O5-C1-C2	-2.29	107.14	110.86
3	C	504	NAG	C2-N2-C7	-2.22	120.19	123.04
10	B	501	NAG	C2-N2-C7	-2.17	120.25	123.04
4	A	516	FUL	C1-C2-C3	-2.13	107.03	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	514	MAN	O5-C1-C2	-2.10	107.45	110.86
3	A	508	NAG	C2-N2-C7	-2.09	120.35	123.04
3	C	504	NAG	O3-C3-C2	-2.07	105.01	109.11
3	C	501	NAG	O3-C3-C2	-2.07	105.02	109.11
3	A	501	NAG	C2-N2-C7	-2.06	120.39	123.04
7	C	508	NAG	C2-N2-C7	-2.05	120.41	123.04
7	C	509	FUL	O5-C1-C2	-2.03	107.57	110.86
9	E	506	FUL	O5-C5-C6	2.06	109.54	106.13
5	E	501	NAG	C1-O5-C5	2.07	114.88	112.25
3	C	506	MAN	C1-O5-C5	2.09	114.90	112.25
3	C	502	FUC	O5-C5-C6	2.13	109.66	106.13
10	B	502	FUL	O5-C5-C6	2.17	109.71	106.13
3	A	503	FUL	O5-C5-C6	2.20	109.76	106.13
9	E	505	FUC	O5-C5-C6	2.24	109.83	106.13
3	A	510	FUL	O5-C5-C6	2.31	109.94	106.13
7	C	510	NAG	C3-C4-C5	2.31	114.23	110.20
3	A	509	FUC	O5-C5-C6	2.32	109.97	106.13
3	A	502	FUC	O5-C5-C6	2.40	110.10	106.13
10	B	501	NAG	C4-C3-C2	2.42	114.99	111.23
7	C	510	NAG	O5-C5-C6	2.46	112.67	107.35
7	C	512	BMA	C1-C2-C3	2.48	112.47	109.54
3	C	503	FUL	O5-C5-C6	2.57	110.37	106.13
3	C	501	NAG	C1-O5-C5	2.74	115.72	112.25
4	A	515	NAG	C4-C3-C2	2.81	115.60	111.23
5	D	502	NAG	C3-C4-C5	2.83	115.14	110.20
10	B	501	NAG	C3-C4-C5	2.88	115.22	110.20
3	A	512	BMA	C1-O5-C5	3.00	116.05	112.25
5	D	502	NAG	C1-O5-C5	3.90	117.20	112.25
9	E	505	FUC	C1-O5-C5	4.25	118.94	112.38
9	E	505	FUC	C1-C2-C3	4.70	115.11	109.54
5	E	508	NAG	C3-C4-C5	4.92	118.77	110.20
7	C	510	NAG	C1-O5-C5	5.08	118.69	112.25

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	507	MAN	C1-C2-C3-C4-C5-O5

9 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	FUC	1	0
3	A	512	BMA	1	0
3	A	514	MAN	1	0
3	C	502	FUC	1	0
3	C	504	NAG	2	0
3	C	505	BMA	1	0
3	C	507	MAN	3	0
9	E	504	NAG	2	0
9	E	505	FUC	1	0

5.6 Ligand geometry (i)

14 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	$\#\|Z\| > 2$
6	P4G	A	521	-	10,10,10	0.69	0	9,9,9	1.31	0
6	P4G	B	504	-	10,10,10	0.66	0	9,9,9	1.47	1 (11%)
6	P4G	B	505	-	10,10,10	0.69	0	9,9,9	1.55	2 (22%)
6	P4G	B	506	-	10,10,10	0.67	0	9,9,9	1.61	3 (33%)
8	NAG	C	513	1	14,14,15	0.49	0	15,19,21	0.96	2 (13%)
6	P4G	C	514	-	10,10,10	0.69	0	9,9,9	1.41	0
6	P4G	C	515	-	10,10,10	0.71	0	9,9,9	1.46	0
6	P4G	C	516	-	10,10,10	0.66	0	9,9,9	1.40	0
6	P4G	D	503	-	10,10,10	0.68	0	9,9,9	1.43	1 (11%)
8	NAG	E	503	1	14,14,15	0.45	0	15,19,21	0.80	0
6	P4G	E	510	-	10,10,10	0.68	0	9,9,9	1.39	0
6	P4G	E	511	-	10,10,10	0.67	0	9,9,9	1.54	2 (22%)
6	P4G	F	503	-	10,10,10	0.69	0	9,9,9	1.49	1 (11%)
6	P4G	F	504	-	10,10,10	0.66	0	9,9,9	1.44	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
6	P4G	A	521	-	-	0/8/8/8	0/0/0/0
6	P4G	B	504	-	-	0/8/8/8	0/0/0/0
6	P4G	B	505	-	-	0/8/8/8	0/0/0/0
6	P4G	B	506	-	-	0/8/8/8	0/0/0/0
8	NAG	C	513	1	-	0/6/23/26	0/1/1/1
6	P4G	C	514	-	-	0/8/8/8	0/0/0/0
6	P4G	C	515	-	-	0/8/8/8	0/0/0/0
6	P4G	C	516	-	-	0/8/8/8	0/0/0/0
6	P4G	D	503	-	-	0/8/8/8	0/0/0/0
8	NAG	E	503	1	-	0/6/23/26	0/1/1/1
6	P4G	E	510	-	-	0/8/8/8	0/0/0/0
6	P4G	E	511	-	-	0/8/8/8	0/0/0/0
6	P4G	F	503	-	-	0/8/8/8	0/0/0/0
6	P4G	F	504	-	-	0/8/8/8	0/0/0/0

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	513	NAG	C2-N2-C7	-2.23	120.17	123.04
6	B	506	P4G	C2-O2-C3	2.03	120.58	112.80
6	B	506	P4G	O3-C5-C6	2.04	119.41	110.36
6	D	503	P4G	C2-O2-C3	2.07	120.74	112.80
6	E	511	P4G	C7-O4-C6	2.08	120.77	112.80
6	B	505	P4G	C7-O4-C6	2.12	120.90	112.80
6	B	506	P4G	O4-C6-C5	2.12	119.79	110.36
6	B	504	P4G	C7-O4-C6	2.13	120.97	112.80
6	B	505	P4G	C2-O2-C3	2.16	121.08	112.80
6	E	511	P4G	C4-O3-C5	2.32	123.28	113.31
8	C	513	NAG	C1-O5-C5	2.35	115.23	112.25
6	F	503	P4G	C7-O4-C6	2.38	121.90	112.80

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	A	521	P4G	1	0
6	C	515	P4G	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	322/329 (97%)	-0.11	8 (2%) 61 68	30, 45, 70, 110	0
1	C	322/329 (97%)	-0.38	0 100 100	26, 38, 56, 95	0
1	E	322/329 (97%)	-0.31	2 (0%) 90 92	28, 43, 69, 94	0
2	B	170/181 (93%)	-0.13	0 100 100	27, 40, 62, 84	0
2	D	170/181 (93%)	-0.07	2 (1%) 81 85	27, 43, 69, 79	0
2	F	170/181 (93%)	-0.16	0 100 100	26, 40, 62, 77	0
All	All	1476/1530 (96%)	-0.22	12 (0%) 87 90	26, 42, 67, 110	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	142(A)	THR	3.7
1	A	173	ASN	3.5
1	A	142	ASP	2.9
1	A	326	LYS	2.9
1	A	143	ASN	2.5
1	A	141	TYR	2.2
1	E	141	TYR	2.2
2	D	73	ILE	2.2
1	A	144	GLY	2.2
1	E	126	ARG	2.2
1	A	222	ILE	2.2
2	D	84	VAL	2.0

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

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
9	FUC	E	505	10/11	0.62	0.33	18.18	60,85,92,92	0
3	MAN	C	507	11/12	0.70	0.28	13.66	68,94,104,108	0
9	NAG	E	507	14/15	0.78	0.28	7.16	71,85,96,97	0
4	NAG	A	515	14/15	0.88	0.15	4.11	51,68,85,92	0
9	NAG	E	504	14/15	0.86	0.16	2.23	60,69,89,89	0
5	NAG	D	501	14/15	0.81	0.18	2.14	77,99,111,112	0
3	MAN	A	507	11/12	0.88	0.17	1.77	52,59,65,69	0
10	FUL	B	502	10/11	0.64	0.54	-	116,119,123,124	0
5	NAG	D	502	14/15	0.81	0.27	-	118,123,127,128	0
3	NAG	A	504	14/15	0.97	0.12	-	54,62,66,67	0
3	MAN	C	506	11/12	0.69	0.34	-	105,118,122,122	0
7	NAG	C	510	14/15	0.81	0.17	-	59,74,85,92	0
3	MAN	A	513	11/12	0.85	0.38	-	72,83,90,90	0
4	FUL	A	516	10/11	0.83	0.19	-	82,92,94,97	0
7	BMA	C	512	11/12	0.64	0.21	-	92,103,110,115	0
3	BMA	A	512	11/12	0.85	0.25	-	60,67,71,81	0
3	NAG	A	508	14/15	0.88	0.23	-	59,74,82,92	0
10	NAG	B	503	14/15	0.80	0.37	-	95,103,110,114	0
3	MAN	A	514	11/12	0.63	0.49	-	98,109,113,114	0
3	FUL	A	503	10/11	0.88	0.16	-	67,77,82,92	0
3	FUL	C	503	10/11	0.81	0.18	-	74,79,90,97	0
3	NAG	A	511	14/15	0.92	0.18	-	63,66,75,86	0
5	NAG	E	509	14/15	0.62	0.42	-	126,131,140,142	0
5	NAG	F	501	14/15	0.87	0.20	-	83,99,106,116	0
3	FUC	C	502	10/11	0.90	0.14	-	62,66,70,71	0
5	NAG	F	502	14/15	0.77	0.46	-	118,130,134,135	0
7	FUL	C	509	10/11	0.92	0.17	-	45,77,80,80	0
5	NAG	E	508	14/15	0.66	0.22	-	90,102,111,121	0
3	FUC	A	509	10/11	0.86	0.38	-	95,105,109,109	0
9	FUL	E	506	10/11	0.73	0.42	-	110,122,126,128	0
3	MAN	A	506	11/12	0.82	0.31	-	78,85,97,100	0
5	NAG	E	501	14/15	0.81	0.28	-	81,94,105,117	0
3	FUL	A	510	10/11	0.65	0.50	-	101,109,119,121	0
3	NAG	A	501	14/15	0.94	0.12	-	39,45,55,56	0
4	FUL	A	517	10/11	0.75	0.41	-	95,103,114,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	FUC	A	502	10/11	0.89	0.16	-	55,65,69,74	0
5	NAG	E	502	14/15	0.67	0.40	-	114,124,129,129	0
5	NAG	A	519	14/15	0.82	0.18	-	69,79,91,106	0
7	NAG	C	508	14/15	0.92	0.12	-	47,57,74,77	0
3	BMA	C	505	11/12	0.80	0.16	-	72,74,84,85	0
3	NAG	C	504	14/15	0.94	0.09	-	44,56,72,74	0
3	BMA	A	505	11/12	0.86	0.11	-	52,63,68,70	0
4	NAG	A	518	14/15	0.75	0.24	-	72,98,112,113	0
10	NAG	B	501	14/15	0.78	0.17	-	75,84,97,108	0
3	NAG	C	501	14/15	0.90	0.08	-	39,45,54,60	0
7	BMA	C	511	11/12	0.70	0.16	-	100,104,108,109	0
5	NAG	A	520	14/15	0.75	0.35	-	118,124,127,128	0

6.4 Ligands

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	P4G	F	504	11/11	0.64	0.33	11.68	74,81,89,90	0
6	P4G	B	506	11/11	0.62	0.39	9.52	74,82,92,92	0
6	P4G	E	511	11/11	0.79	0.17	8.05	47,62,74,74	0
6	P4G	C	515	11/11	0.81	0.24	6.41	52,70,88,92	0
6	P4G	B	505	11/11	0.84	0.19	6.19	61,69,88,91	0
6	P4G	A	521	11/11	0.82	0.33	5.49	69,81,93,94	0
6	P4G	F	503	11/11	0.80	0.22	4.95	60,72,99,101	0
8	NAG	C	513	14/15	0.88	0.17	2.56	67,81,90,94	0
6	P4G	D	503	11/11	0.79	0.20	2.30	64,68,89,90	0
6	P4G	C	514	11/11	0.92	0.10	1.11	55,62,69,73	0
6	P4G	B	504	11/11	0.94	0.12	0.88	35,59,72,74	0
8	NAG	E	503	14/15	0.62	0.30	-	96,110,117,117	0
6	P4G	E	510	11/11	0.86	0.17	-	75,90,98,99	0
6	P4G	C	516	11/11	0.79	0.22	-	89,97,100,106	0

6.5 Other polymers

There are no such residues in this entry.