



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:24 PM GMT

PDB ID : 4I78
Title : Crystal structure of a subtype H17 hemagglutinin homologue from A/little yellow-shouldered bat/Guatemala/060/2010 (H17N10)
Authors : Zhu, X.; Wilson, I.A.
Deposited on : 2012-11-30
Resolution : 3.18 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 ⓘ symbol.

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

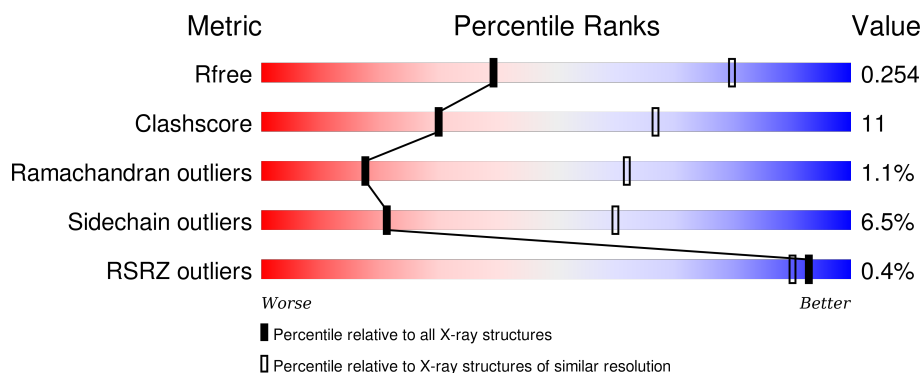
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 3.18 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	1115 (3.22-3.14)
Clashscore	102246	1125 (3.20-3.16)
Ramachandran outliers	100387	1105 (3.20-3.16)
Sidechain outliers	100360	1104 (3.20-3.16)
RSRZ outliers	91569	1120 (3.22-3.14)

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 $\leq 5\%$. 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	328	 70% 23% • •
1	B	328	 72% 21% • •
2	C	181	 77% 13% • • 6%
2	D	181	 78% 13% • • 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7816 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	319	Total	C	N	O	S	0	0	0
			2512	1579	431	489	13			
1	B	319	Total	C	N	O	S	0	0	0
			2512	1579	431	489	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	EXPRESSION TAG	UNP H6QM93
A	8	ASP	-	EXPRESSION TAG	UNP H6QM93
A	9	PRO	-	EXPRESSION TAG	UNP H6QM93
B	7	ALA	-	EXPRESSION TAG	UNP H6QM93
B	8	ASP	-	EXPRESSION TAG	UNP H6QM93
B	9	PRO	-	EXPRESSION TAG	UNP H6QM93

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	170	Total	C	N	O	S	0	0	0
			1377	859	236	275	7			
2	D	170	Total	C	N	O	S	0	0	0
			1377	859	236	275	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	47	GLY	ALA	ENGINEERED MUTATION	UNP H6QM93
C	175	SER	-	EXPRESSION TAG	UNP H6QM93
C	176	GLY	-	EXPRESSION TAG	UNP H6QM93
C	177	ARG	-	EXPRESSION TAG	UNP H6QM93
C	178	LEU	-	EXPRESSION TAG	UNP H6QM93
C	179	VAL	-	EXPRESSION TAG	UNP H6QM93

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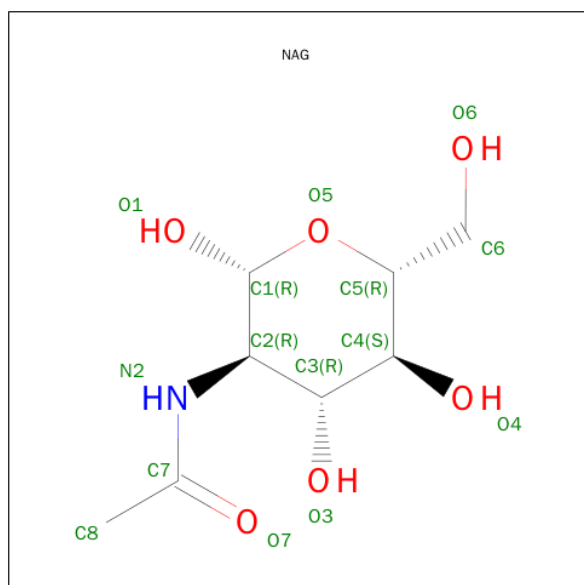
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Chain	Residue	Modelled	Actual	Comment	Reference
C	180	PRO	-	EXPRESSION TAG	UNP H6QM93
C	181	ARG	-	EXPRESSION TAG	UNP H6QM93
D	47	GLY	ALA	ENGINEERED MUTATION	UNP H6QM93
D	175	SER	-	EXPRESSION TAG	UNP H6QM93
D	176	GLY	-	EXPRESSION TAG	UNP H6QM93
D	177	ARG	-	EXPRESSION TAG	UNP H6QM93
D	178	LEU	-	EXPRESSION TAG	UNP H6QM93
D	179	VAL	-	EXPRESSION TAG	UNP H6QM93
D	180	PRO	-	EXPRESSION TAG	UNP H6QM93
D	181	ARG	-	EXPRESSION TAG	UNP H6QM93

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

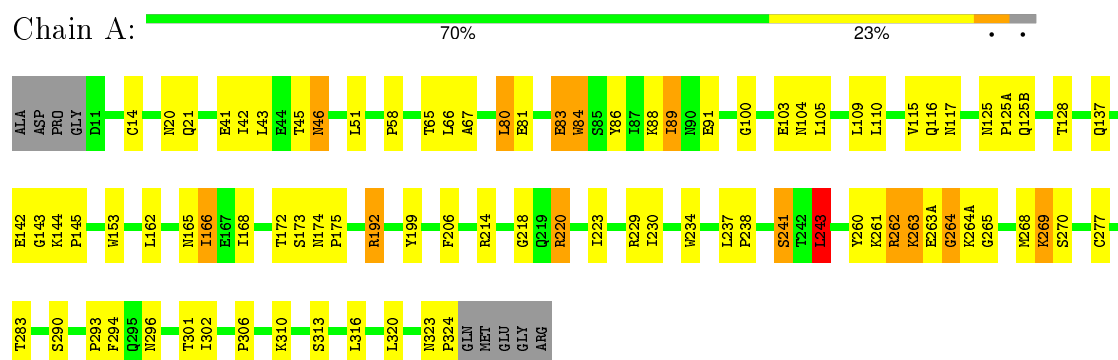


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

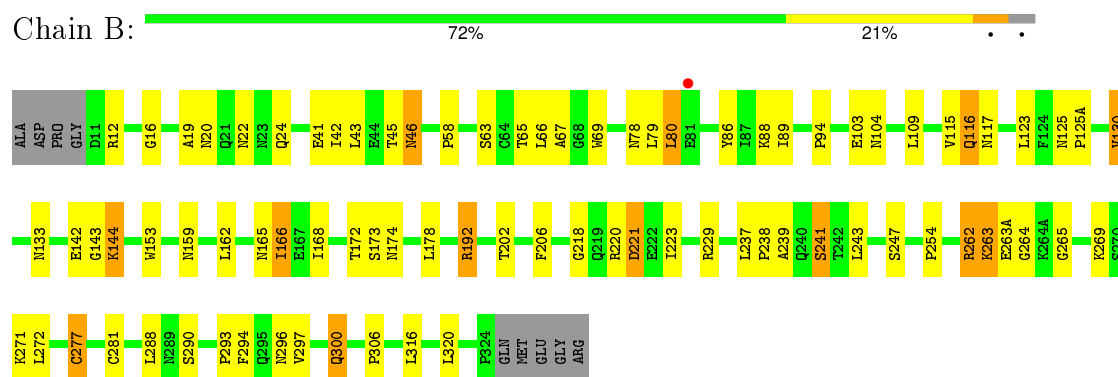
3 Residue-property plots [i](#)

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.

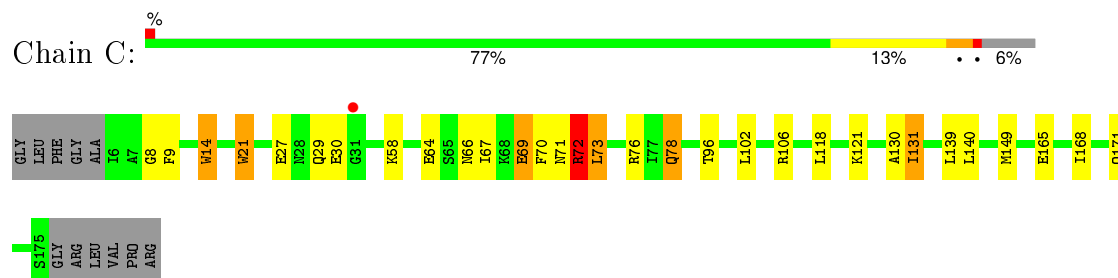
• Molecule 1: Hemagglutinin HA1



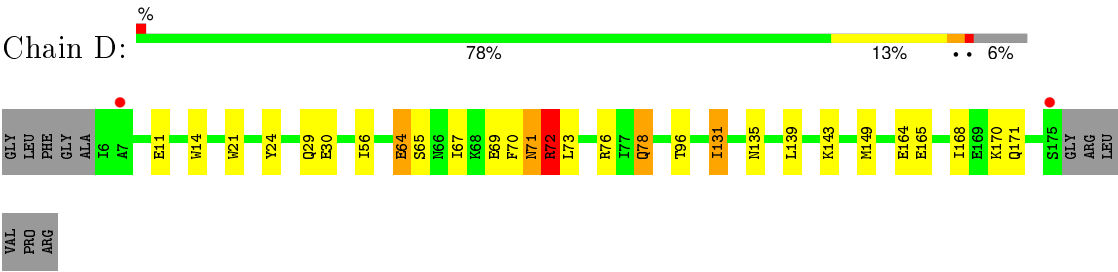
• Molecule 1: Hemagglutinin HA1



• Molecule 2: Hemagglutinin HA2



• Molecule 2: Hemagglutinin HA2



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	100.83Å 100.83Å 760.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.18 49.44 – 3.18	Depositor EDS
% Data completeness (in resolution range)	96.1 (50.00-3.18) 96.3 (49.44-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.203 , 0.258 0.201 , 0.254	Depositor DCC
R_{free} test set	1250 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	64.7	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 24987 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7816	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: NAG, FUC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.69	2/2569 (0.1%)	0.84	1/3493 (0.0%)
1	B	0.68	2/2569 (0.1%)	0.83	1/3493 (0.0%)
2	C	0.64	2/1401 (0.1%)	0.74	2/1884 (0.1%)
2	D	0.64	1/1401 (0.1%)	0.76	1/1884 (0.1%)
All	All	0.67	7/7940 (0.1%)	0.81	5/10754 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	14	TRP	CD2-CE2	5.84	1.48	1.41
1	B	153	TRP	CD2-CE2	5.61	1.48	1.41
2	C	14	TRP	CD2-CE2	5.60	1.48	1.41
1	A	153	TRP	CD2-CE2	5.35	1.47	1.41
1	A	84	TRP	CD2-CE2	5.34	1.47	1.41
2	C	21	TRP	CD2-CE2	5.17	1.47	1.41
1	B	69	TRP	CD2-CE2	5.13	1.47	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	72	ARG	NE-CZ-NH1	6.18	123.39	120.30
2	C	73	LEU	C-N-CA	-5.90	106.96	121.70
1	B	117	ASN	N-CA-C	-5.67	95.69	111.00
1	A	243	LEU	CA-CB-CG	5.42	127.78	115.30
2	C	72	ARG	N-CA-C	-5.23	96.89	111.00

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	2512	0	2426	65	0
1	B	2512	0	2426	58	0
2	C	1377	0	1306	29	0
2	D	1377	0	1306	28	0
3	A	24	0	22	0	0
4	B	14	0	13	0	0
All	All	7816	0	7499	170	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 11.

All (170) 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:B:116:GLN:HG3	1:B:263:LYS:HD3	1.43	0.99
2:C:67:ILE:HG22	2:C:69:GLU:HG3	1.47	0.96
2:D:67:ILE:HG22	2:D:69:GLU:HG3	1.47	0.96
2:C:72:ARG:O	2:C:73:LEU:HD12	1.70	0.91
1:A:80:LEU:HD12	1:A:80:LEU:H	1.39	0.87
1:A:263(A):GLU:N	1:A:263(A):GLU:OE1	2.11	0.84
2:D:71:ASN:HD22	2:D:78:GLN:CG	1.91	0.83
1:A:206:PHE:HE1	1:A:241:SER:HG	1.26	0.82
2:D:131:ILE:HG23	2:D:139:LEU:HB3	1.61	0.81
2:D:71:ASN:ND2	2:D:78:GLN:HG3	1.95	0.81
2:C:71:ASN:C	2:C:73:LEU:H	1.83	0.80
2:C:131:ILE:HG23	2:C:139:LEU:HB3	1.63	0.80
2:D:71:ASN:ND2	2:D:78:GLN:CG	2.47	0.78
2:D:72:ARG:HH11	2:D:72:ARG:HG3	1.49	0.77
1:B:243:LEU:O	1:B:243:LEU:HD12	1.85	0.77
2:D:71:ASN:HD22	2:D:78:GLN:HG2	1.51	0.76
2:C:71:ASN:C	2:C:73:LEU:N	2.37	0.76
1:B:320:LEU:HD11	2:C:21:TRP:CD1	2.21	0.76
1:B:178:LEU:HD11	1:B:243:LEU:HD21	1.68	0.75
1:A:294:PHE:CE1	2:D:96:THR:HG21	2.23	0.74
1:A:91:GLU:HG2	1:A:269:LYS:HE3	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:GLN:HG3	1:B:263:LYS:CD	2.16	0.73
1:A:192:ARG:HH11	1:A:192:ARG:CG	2.02	0.73
1:A:206:PHE:HE1	1:A:241:SER:OG	1.71	0.72
1:A:80:LEU:HD12	1:A:80:LEU:N	2.04	0.71
2:D:72:ARG:HH11	2:D:72:ARG:CG	2.03	0.71
1:A:91:GLU:CG	1:A:269:LYS:HE3	2.21	0.70
1:A:237:LEU:HD12	1:A:238:PRO:HD2	1.72	0.69
2:C:71:ASN:O	2:C:73:LEU:N	2.22	0.69
1:B:192:ARG:NH1	1:B:192:ARG:HB3	2.08	0.69
2:C:67:ILE:CG2	2:C:69:GLU:HG3	2.20	0.69
1:A:192:ARG:HH11	1:A:192:ARG:HG2	1.58	0.69
1:A:116:GLN:HG3	1:A:263:LYS:HD3	1.75	0.68
2:D:67:ILE:CG2	2:D:69:GLU:HG3	2.24	0.67
1:B:263(A):GLU:N	1:B:263(A):GLU:OE1	2.19	0.67
1:B:19:ALA:O	1:B:20:ASN:OD1	2.13	0.66
1:A:80:LEU:CD1	1:A:80:LEU:H	2.10	0.64
1:B:192:ARG:HH11	1:B:192:ARG:HB3	1.63	0.64
1:A:192:ARG:HH11	1:A:192:ARG:HB3	1.63	0.63
1:A:172:THR:HG22	1:A:174:ASN:H	1.63	0.62
1:A:262:ARG:H	1:A:262:ARG:NE	1.98	0.62
1:A:263(A):GLU:HG2	1:A:264:GLY:H	1.62	0.62
1:B:243:LEU:HD12	1:B:243:LEU:C	2.19	0.62
1:A:192:ARG:NH1	1:A:192:ARG:HB3	2.14	0.62
2:C:76:ARG:HH11	2:C:76:ARG:HG3	1.65	0.62
1:B:192:ARG:HH11	1:B:192:ARG:CG	2.13	0.61
1:A:223:ILE:HD13	1:A:229:ARG:HH22	1.65	0.61
1:A:192:ARG:HH11	1:A:192:ARG:CB	2.13	0.60
1:B:192:ARG:CB	1:B:192:ARG:HH11	2.14	0.60
1:A:218:GLY:O	1:A:220:ARG:NH1	2.34	0.60
1:B:178:LEU:HD11	1:B:243:LEU:CD2	2.31	0.59
1:B:290:SER:HB2	1:B:306:PRO:HD3	1.84	0.58
2:D:64:GLU:HG3	2:D:65:SER:N	2.18	0.58
1:B:79:LEU:O	1:B:80:LEU:O	2.22	0.58
1:A:89:ILE:HG22	1:A:269:LYS:HG2	1.84	0.58
1:B:288:LEU:HD21	1:B:297:VAL:HG21	1.84	0.58
1:A:165:ASN:C	1:A:166:ILE:HG12	2.23	0.57
1:A:51:LEU:HD11	1:A:270:SER:HB3	1.87	0.57
2:D:71:ASN:HD21	2:D:78:GLN:HG3	1.68	0.57
1:B:178:LEU:CD1	1:B:243:LEU:HD21	2.35	0.57
1:B:206:PHE:HE1	1:B:241:SER:OG	1.88	0.56
1:B:63:SER:O	1:B:94:PRO:HD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:130:ALA:HB2	2:C:140:LEU:HD23	1.86	0.56
2:D:29:GLN:HG2	2:D:30:GLU:OE1	2.06	0.56
1:B:223:ILE:HD13	1:B:229:ARG:HH22	1.71	0.56
1:B:42:ILE:O	1:B:293:PRO:HD2	2.06	0.56
1:B:165:ASN:C	1:B:166:ILE:HG12	2.27	0.55
1:A:116:GLN:HG3	1:A:263:LYS:CD	2.36	0.55
1:B:46:ASN:N	1:B:46:ASN:OD1	2.39	0.55
1:A:20:ASN:OD1	1:A:21:GLN:N	2.39	0.55
2:C:72:ARG:C	2:C:73:LEU:HD12	2.26	0.55
2:C:8:GLY:HA2	2:C:14:TRP:HZ2	1.72	0.54
1:A:43:LEU:HD23	1:A:313:SER:HA	1.90	0.54
1:A:83:GLU:HG3	1:A:84:TRP:N	2.22	0.54
2:C:29:GLN:HG2	2:C:30:GLU:OE1	2.08	0.53
1:B:300:GLN:HG3	2:C:66:ASN:HB3	1.90	0.53
1:B:262:ARG:H	1:B:262:ARG:NE	2.05	0.53
2:D:70:PHE:O	2:D:70:PHE:CD1	2.61	0.53
1:A:263(A):GLU:O	1:A:264(A):LYS:N	2.42	0.53
1:B:218:GLY:O	1:B:220:ARG:NH1	2.42	0.52
1:A:116:GLN:HG3	1:A:263:LYS:HE2	1.92	0.52
1:B:88:LYS:HE2	1:B:272:LEU:O	2.09	0.52
1:A:117:ASN:O	1:A:260:TYR:HA	2.10	0.52
1:A:223:ILE:HD13	1:A:229:ARG:NH2	2.25	0.51
1:B:22:ASN:HD21	1:B:24:GLN:HB2	1.74	0.51
1:B:206:PHE:HE1	1:B:241:SER:HG	1.56	0.51
1:A:142:GLU:C	1:A:144:LYS:H	2.14	0.51
2:C:102:LEU:O	2:C:106:ARG:HG3	2.10	0.51
2:C:76:ARG:NH1	2:C:76:ARG:HG3	2.24	0.51
1:A:91:GLU:HG3	1:A:269:LYS:HE3	1.93	0.51
1:B:65:THR:HG22	1:B:67:ALA:H	1.76	0.50
1:A:46:ASN:OD1	1:A:46:ASN:N	2.44	0.50
1:A:268:MET:HE2	1:A:302:ILE:HD12	1.94	0.50
1:B:66:LEU:HD23	1:B:109:LEU:HD12	1.93	0.50
1:B:192:ARG:HH11	1:B:192:ARG:HG2	1.76	0.49
1:B:22:ASN:ND2	1:B:24:GLN:HB2	2.28	0.49
1:A:294:PHE:CZ	2:D:96:THR:HG21	2.47	0.49
1:B:172:THR:HG22	1:B:174:ASN:H	1.77	0.49
1:A:58:PRO:HB3	1:A:86:TYR:CZ	2.48	0.49
1:A:65:THR:HG22	1:A:67:ALA:H	1.77	0.48
2:D:72:ARG:O	2:D:72:ARG:HG3	2.14	0.48
1:A:172:THR:HG22	1:A:173:SER:N	2.29	0.48
1:B:168:ILE:HD13	1:B:243:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ARG:H	1:A:262:ARG:HE	1.60	0.48
1:B:79:LEU:HD12	1:B:80:LEU:H	1.78	0.48
1:A:174:ASN:HB3	1:A:175:PRO:HD2	1.96	0.48
1:A:320:LEU:HD11	2:D:21:TRP:CD1	2.49	0.47
1:A:104:ASN:HB3	1:A:234:TRP:HE1	1.79	0.47
2:D:78:GLN:NE2	2:D:78:GLN:HA	2.14	0.47
1:B:173:SER:HA	1:B:239:ALA:HB1	1.96	0.47
1:A:290:SER:HB2	1:A:306:PRO:HD3	1.96	0.47
1:A:45:THR:HG22	1:A:296:ASN:OD1	2.14	0.47
1:B:281:CYS:SG	1:B:288:LEU:HD12	2.54	0.47
2:C:71:ASN:HB3	2:C:73:LEU:HB2	1.97	0.47
1:B:144:LYS:HD2	1:B:144:LYS:HA	1.61	0.47
2:C:168:ILE:O	2:C:171:GLN:HG2	2.15	0.47
1:A:105:LEU:HG	1:A:109:LEU:HD13	1.97	0.46
1:A:42:ILE:O	1:A:293:PRO:HD2	2.15	0.46
1:B:12:ARG:HB2	2:C:27:GLU:HB3	1.97	0.46
2:D:72:ARG:NH1	2:D:72:ARG:HG3	2.25	0.46
2:C:58:LYS:HD3	2:C:58:LYS:HA	1.65	0.46
1:A:65:THR:HG22	1:A:66:LEU:N	2.30	0.46
2:C:70:PHE:HD1	2:C:70:PHE:O	1.99	0.46
1:B:290:SER:CB	1:B:306:PRO:HD3	2.46	0.46
1:A:293:PRO:HG3	2:D:56:ILE:HA	1.97	0.46
1:B:263(A):GLU:CD	1:B:263(A):GLU:H	2.13	0.46
1:B:125:ASN:HA	1:B:125(A):PRO:HD3	1.83	0.45
2:C:168:ILE:HA	2:C:171:GLN:HE21	1.80	0.45
1:B:58:PRO:HB3	1:B:86:TYR:CZ	2.51	0.45
1:A:14:CYS:O	2:D:24:TYR:HA	2.17	0.45
2:C:165:GLU:O	2:C:168:ILE:HG13	2.17	0.45
1:A:323:ASN:HA	1:A:324:PRO:HD2	1.85	0.45
2:D:165:GLU:O	2:D:168:ILE:HG13	2.17	0.45
1:A:168:ILE:HB	1:A:243:LEU:HD12	1.99	0.44
2:D:71:ASN:C	2:D:73:LEU:N	2.70	0.44
1:A:100:GLY:HA3	1:A:230:ILE:O	2.18	0.44
1:B:130:VAL:HG23	1:B:159:ASN:HB3	1.99	0.44
1:B:172:THR:HG22	1:B:173:SER:N	2.32	0.44
2:C:78:GLN:NE2	2:C:78:GLN:HA	2.19	0.44
1:B:237:LEU:HD12	1:B:238:PRO:HD2	1.99	0.43
2:D:168:ILE:O	2:D:171:GLN:HG2	2.18	0.43
1:A:89:ILE:CG2	1:A:269:LYS:HG2	2.48	0.43
1:B:142:GLU:C	1:B:144:LYS:H	2.22	0.43
1:B:16:GLY:HA2	2:C:9:PHE:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:11:GLU:OE2	2:D:135:ASN:HB2	2.19	0.42
1:B:41:GLU:OE2	1:B:43:LEU:HB3	2.19	0.42
1:A:41:GLU:OE2	1:A:43:LEU:HB3	2.20	0.42
1:A:199:TYR:CE2	1:A:214:ARG:HD3	2.54	0.42
1:B:294:PHE:CE1	2:C:96:THR:HG21	2.54	0.42
1:A:116:GLN:HG3	1:A:263:LYS:CE	2.49	0.42
1:B:263(A):GLU:HG2	1:B:264:GLY:H	1.85	0.42
1:B:202:THR:HG23	1:B:247:SER:HB2	2.02	0.42
1:B:123:LEU:HD12	1:B:254:PRO:HB2	2.02	0.42
1:A:66:LEU:HD23	1:A:109:LEU:HD12	2.02	0.42
1:A:125:ASN:HA	1:A:125(A):PRO:HD3	1.80	0.42
1:B:45:THR:HG22	1:B:296:ASN:OD1	2.20	0.42
1:B:142:GLU:O	1:B:144:LYS:N	2.51	0.42
1:B:221:ASP:HB3	1:B:223:ILE:CD1	2.50	0.41
1:A:283:THR:HG22	1:A:301:THR:HG22	2.02	0.41
2:D:170:LYS:HA	2:D:170:LYS:HD2	1.89	0.41
1:A:263:LYS:O	1:A:264(A):LYS:HG3	2.20	0.41
2:D:72:ARG:NH1	2:D:72:ARG:CG	2.71	0.41
1:B:78:ASN:O	1:B:79:LEU:C	2.57	0.41
1:A:263:LYS:HG2	1:A:263:LYS:H	1.69	0.41
2:C:72:ARG:HG3	2:C:72:ARG:O	2.20	0.41
2:D:71:ASN:C	2:D:73:LEU:H	2.24	0.41
2:C:121:LYS:HE2	2:C:121:LYS:HB3	1.93	0.41
2:C:30:GLU:OE1	2:C:30:GLU:N	2.45	0.41
1:A:261:LYS:HB3	1:A:261:LYS:HE3	1.81	0.41
1:A:137:GLN:HA	1:A:145:PRO:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	317/328 (97%)	292 (92%)	21 (7%)	4 (1%)	15	58
1	B	317/328 (97%)	295 (93%)	17 (5%)	5 (2%)	12	53
2	C	168/181 (93%)	162 (96%)	5 (3%)	1 (1%)	30	74
2	D	168/181 (93%)	163 (97%)	4 (2%)	1 (1%)	30	74
All	All	970/1018 (95%)	912 (94%)	47 (5%)	11 (1%)	17	62

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	265	GLY
1	B	80	LEU
1	B	265	GLY
1	A	264	GLY
1	B	277	CYS
1	B	133	ASN
1	A	81	GLU
2	D	71	ASN
2	C	72	ARG
1	A	143	GLY
1	B	143	GLY

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	281/287 (98%)	259 (92%)	22 (8%)	16	52
1	B	281/287 (98%)	261 (93%)	20 (7%)	18	56
2	C	149/156 (96%)	143 (96%)	6 (4%)	38	76
2	D	149/156 (96%)	141 (95%)	8 (5%)	27	67
All	All	860/886 (97%)	804 (94%)	56 (6%)	21	60

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	80	LEU
1	A	83	GLU
1	A	88	LYS
1	A	89	ILE
1	A	103	GLU
1	A	110	LEU
1	A	115	VAL
1	A	125(B)	GLN
1	A	128	THR
1	A	162	LEU
1	A	166	ILE
1	A	192	ARG
1	A	220	ARG
1	A	241	SER
1	A	243	LEU
1	A	262	ARG
1	A	263	LYS
1	A	269	LYS
1	A	277	CYS
1	A	310	LYS
1	A	316	LEU
1	B	46	ASN
1	B	89	ILE
1	B	103	GLU
1	B	104	ASN
1	B	115	VAL
1	B	116	GLN
1	B	130	VAL
1	B	144	LYS
1	B	162	LEU
1	B	166	ILE
1	B	192	ARG
1	B	221	ASP
1	B	241	SER
1	B	262	ARG
1	B	263	LYS
1	B	269	LYS
1	B	271	LYS
1	B	277	CYS
1	B	300	GLN
1	B	316	LEU
2	C	64	GLU

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Mol	Chain	Res	Type
2	C	69	GLU
2	C	78	GLN
2	C	118	LEU
2	C	131	ILE
2	C	149	MET
2	D	64	GLU
2	D	72	ARG
2	D	76	ARG
2	D	78	GLN
2	D	131	ILE
2	D	143	LYS
2	D	149	MET
2	D	164	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	B	21	GLN
1	B	22	ASN
1	B	165	ASN
1	B	304	ASN
2	C	78	GLN
2	C	171	GLN
2	D	15	GLN
2	D	71	ASN
2	D	78	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 ⓘ

2 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	401	1,3	14,14,15	0.60	0	15,19,21	1.82	4 (26%)
3	FUC	A	402	3	10,10,11	0.79	0	14,14,16	1.19	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
3	NAG	A	401	1,3	-	0/6/23/26	0/1/1/1
3	FUC	A	402	3	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	NAG	O6-C6-C5	-2.12	104.32	111.33
3	A	401	NAG	C4-C3-C2	2.07	114.44	111.23
3	A	402	FUC	O5-C5-C6	2.08	109.57	106.13
3	A	402	FUC	C1-O5-C5	2.13	115.67	112.38
3	A	401	NAG	C3-C4-C5	3.08	115.56	110.20
3	A	401	NAG	C1-O5-C5	4.91	118.48	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

1 ligand is 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	B	401	1	14,14,15	0.52	0	15,19,21	1.73	6 (40%)

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	B	401	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	NAG	O7-C7-C8	-2.31	117.82	122.06
4	B	401	NAG	C4-C3-C2	-2.21	107.79	111.23
4	B	401	NAG	O7-C7-N2	2.15	126.24	121.86
4	B	401	NAG	C2-N2-C7	2.37	126.08	123.04
4	B	401	NAG	O5-C5-C6	2.82	113.44	107.35
4	B	401	NAG	C1-O5-C5	3.06	116.13	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	319/328 (97%)	-0.20	0 100 100	29, 49, 85, 127	0
1	B	319/328 (97%)	-0.28	1 (0%) 94 93	31, 51, 87, 122	0
2	C	170/181 (93%)	0.25	1 (0%) 90 84	31, 87, 129, 168	0
2	D	170/181 (93%)	0.06	2 (1%) 81 69	39, 82, 121, 156	0
All	All	978/1018 (96%)	-0.10	4 (0%) 93 90	29, 56, 115, 168	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	81	GLU	2.9
2	C	31	GLY	2.6
2	D	175	SER	2.3
2	D	7	ALA	2.1

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, 95th 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	A	401	14/15	0.74	0.23	-0.67	104,115,129,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	FUC	A	402	10/11	0.73	0.31	-	108,127,145,151	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, 95th 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(\AA^2)	Q<0.9
4	NAG	B	401	14/15	0.74	0.24	-	90,100,113,136	0

6.5 Other polymers [i](#)

There are no such residues in this entry.