W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2020 – 03:12 PM BST

PDB ID	:	6EA7
Title	:	Structure of EBOV GPcl in complex with the pan-ebolavirus mAb ADI-15878
Authors	:	West, B.R.; Moyer, C.L.; King, L.B.; Fusco, M.L.; Milligan, J.C.; Hui, S.; Saphire, E.O.
Deposited on	:	2018-08-02
Resolution	:	4.25 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 4.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
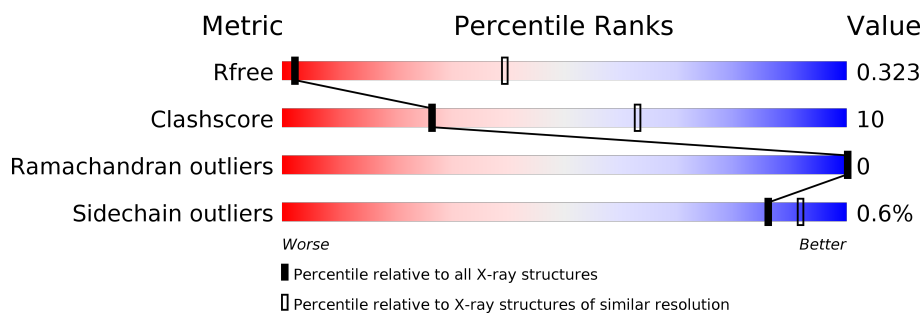
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1017 (4.72-3.78)
Clashscore	141614	1059 (4.72-3.80)
Ramachandran outliers	138981	1014 (4.72-3.80)
Sidechain outliers	138945	1018 (4.72-3.78)

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 respectively. 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%

Mol	Chain	Length	Quality of chain
1	A	163	75% 25%
1	C	163	75% 23% •
1	E	163	77% 19% •
2	B	111	73% 23% 5%
2	D	111	76% 18% 6%
2	F	111	77% 16% 7%
3	H	233	73% 18% 9%

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Mol	Chain	Length	Quality of chain
3	M	233	70% 23% 7%
3	Q	233	73% 21% 5%
4	L	213	80% 18%
4	N	213	80% 19%
4	R	213	78% 20%
5	G	3	67% 33%
6	I	8	38% 63%
6	J	8	25% 63% 13%
7	K	7	57% 14% 29%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 16154 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 Envelope glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	0	0	0
			1252	798	218	231	5			
1	C	159	Total	C	N	O	S	0	0	0
			1213	770	213	225	5			
1	E	156	Total	C	N	O	S	0	0	0
			1190	756	208	221	5			

- Molecule 2 is a protein called Envelope glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	106	Total	C	N	O	S	0	0	0
			830	530	144	150	6			
2	D	104	Total	C	N	O	S	0	0	0
			816	522	141	147	6			
2	F	103	Total	C	N	O	S	0	0	0
			809	517	140	146	6			

- Molecule 3 is a protein called ADI-15878 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	213	Total	C	N	O	S	0	0	0
			1598	1016	269	307	6			
3	M	217	Total	C	N	O	S	0	0	0
			1625	1031	274	314	6			
3	Q	222	Total	C	N	O	S	0	0	0
			1655	1047	280	322	6			

- Molecule 4 is a protein called ADI-15878 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	210	Total	C	N	O	S	0	0	0
			1597	999	261	333	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	211	Total	C	N	O	S	0	0	0
			1606	1005	263	334	4			
4	R	211	Total	C	N	O	S	0	0	0
			1608	1006	266	332	4			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.
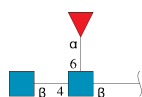
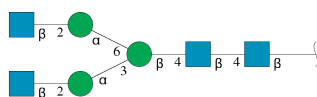| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 6 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
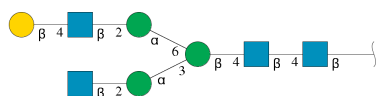
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	8	Total	C	N	O	0	0	0
			100	56	4	40			
6	J	8	Total	C	N	O	0	0	0
			100	56	4	40			

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
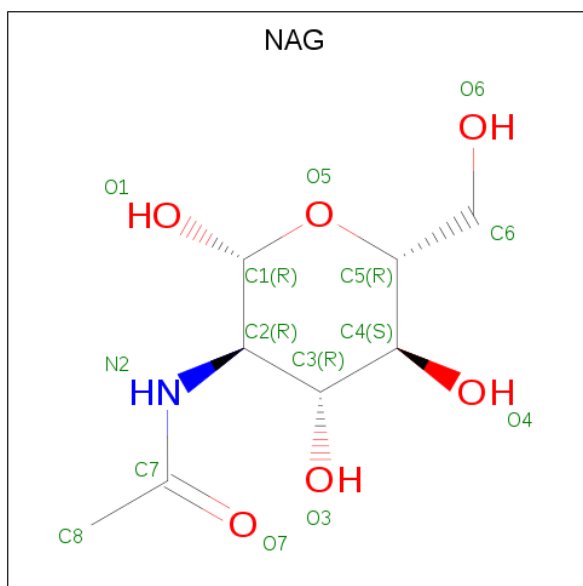
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	K	7	Total 89	C 50	N 4	O 35	0	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

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

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Envelope glycoprotein
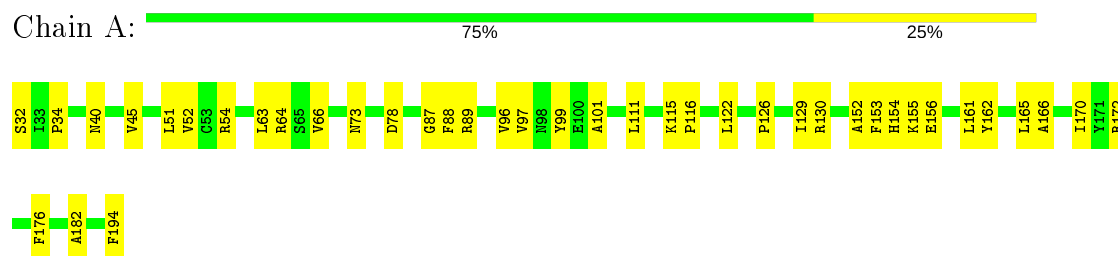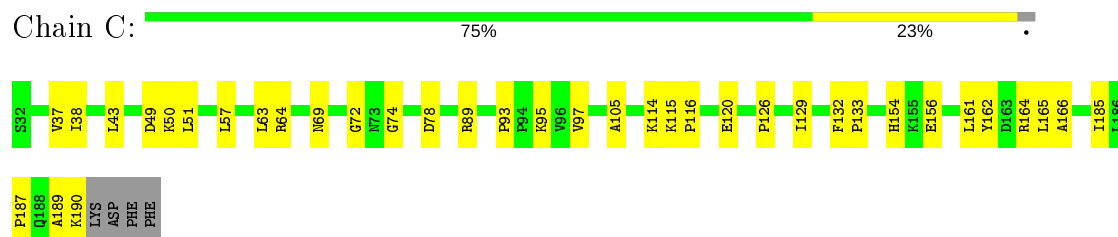
Chain A:

- Molecule 1: Envelope glycoprotein

Chain C:

- Molecule 1: Envelope glycoprotein

Chain E:

- Molecule 2: Envelope glycoprotein

Chain B:

- Molecule 2: Envelope glycoprotein

Chain D:

GLU ALA ILE VAL ASN ALA GLN P509 K510 L515 W531 I532 P533 P537 A538 I542 Y543 M548 Q551 L554 G557 L558 R559 Q560 Q567 R574 E578 L593 L594 Q595 R596 W597 P612
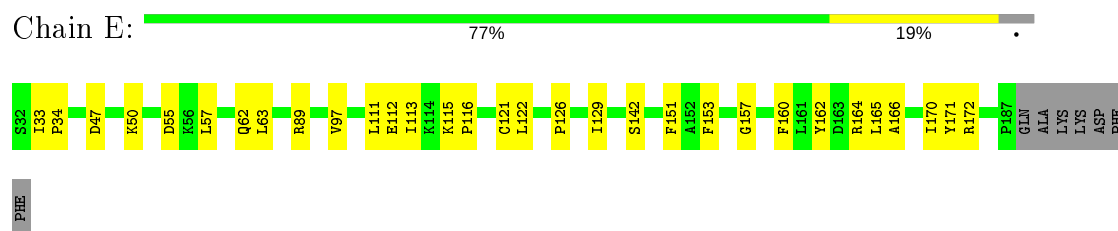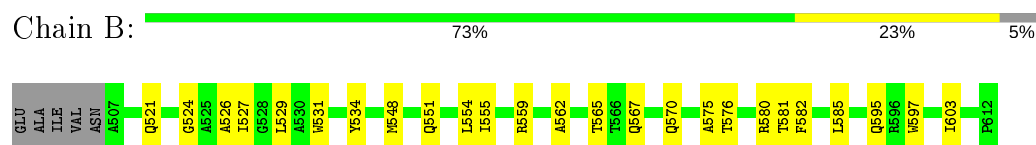
• Molecule 2: Envelope glycoprotein

Chain F: 77%   16%   7%

GLU ALA ILE VAL ASN ALA GLN PRO K510 Q521 D522 E523 G524 A525 A526 I527 W531 P537 I542 Y543 I544 T565 F572 T577 L585 N586 R587 K588 L594 Q595 R596 W597 P612

• Molecule 3: ADI-15878 Fab Heavy Chain

Chain H: 73%   18%   9%

GLN V2 Q3 L4 V5 Q6 P14 G15 F29 M34 S35 A40 K43 V48 I51 S52 G53 L54 A61 V64 F68 T69 I70 S71 R72 M83 N84 S85 L86 T91 K98 D99 H100 H108 F109 D110 Y111 W112 G113 Q114 T119 S122 P128

P135 SER SER LYS SER THR SER GLY GLY T144 L147 D153 Y154 E157 P158 N164 A167 F175 L184 V220 E221 P222 LYS SER CYS ASP LEU GLU VAL ASP ASP ASP
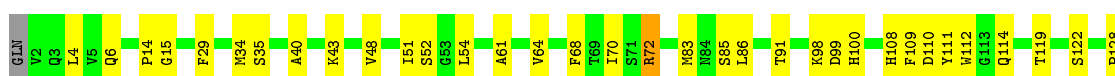
• Molecule 3: ADI-15878 Fab Heavy Chain

Chain M: 70%   23%   7%

GLN V2 T10 Q13 P14 L18 C22 F27 T28 F29 S35 W36 A40 K43 I51 Y59 Y60 A61 V64 K65 G66 R67 F68 T69 I70 S71 R72 D73 K76 L79 Y80 L81 Q82 M83 L86 R87 T91 D99 H100 R101 V102 W103 H108

F109 D110 Y111 Q114 T119 S122 P128 P132 P135 S136 S137 LYS SER THR SER GLY GLY T144 L147 Y154 N164 A167 F175 V190 V193 T202 Y203 K219 V220 E221 P222 K223 S224 CYS ASP LEU GLU VAL ASP ASP ASP

• Molecule 3: ADI-15878 Fab Heavy Chain

Chain Q: 73%   21%   • 5%

Q1 V5 Q6 V12 Q13 P14 C22 F27 M34 S35 W36 A40 K43 G44 L45 S52 A61 V64 R67 F68 R72 L79 Y80 L81 Q82 M83 L86 D90 A97 K98 D99 H100 R101 V102 G106 Y107 H108 F109 D110 Y111 Q114

V120 S121 S122 P128 P135 Y154 F155 P156 W163 N164 A167 L168 F175 V191 T192 V193 T202 Y203 I204 C205 H209 K210 P211 K219 P222 LYS SER CYS ASP LEU GLU VAL ASP ASP ASP

• Molecule 4: ADI-15878 Fab Light Chain

Chain L: 80%   18%   •

D1 I2 V3 L4 T5 Q6 S7 P8 Q27 W32 L33 A34 W35 Y36 I48 S63 L73 C88 Q89 Q90 Y91 Y92 Y93 S94 P95 K102 I105 LYS ARG T108 P112 Q123 T128 N137 F138 Y139 P140 R141 K144 W147 Q154 N157 T163

E164 Q165 T171 Y172 S176 T196 H197 E212 CYS
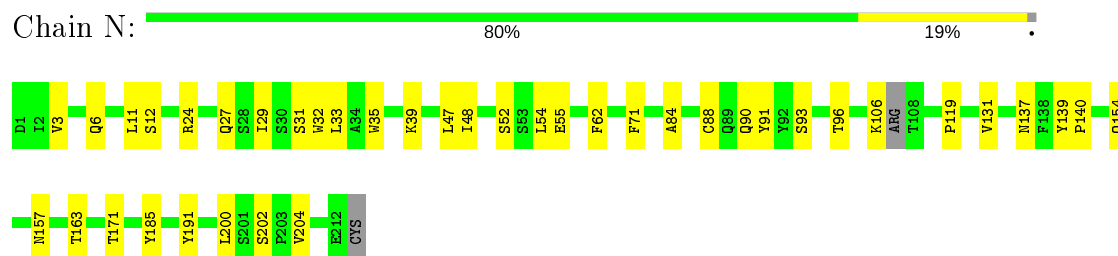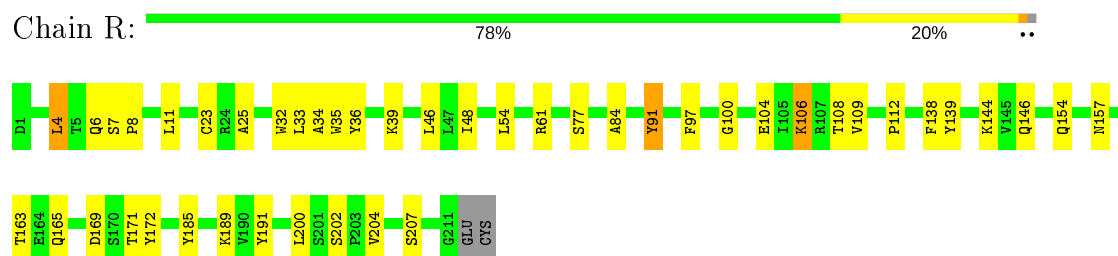
● Molecule 4: ADI-15878 Fab Light Chain

Chain N:

● Molecule 4: ADI-15878 Fab Light Chain

Chain R:

● Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-ace
tamido-2-deoxy-beta-D-glucopyranose

Chain G:

● Molecule 6: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alp
ha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyr
anose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acet
amido-2-deoxy-beta-D-glucopyranose

Chain I:

● Molecule 6: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alp
ha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyr
anose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acet
amido-2-deoxy-beta-D-glucopyranose

Chain J:
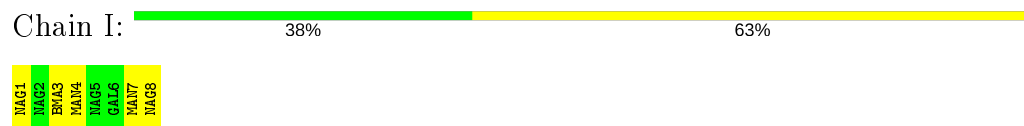
● Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-
acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyra

nose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopy
ranose

Chain K:

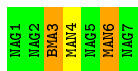57%   14%   29%

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	152.78Å 152.78Å 247.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	56.08 – 4.25 90.42 – 4.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (56.08-4.25) 100.0 (90.42-4.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 4.30Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.280 , 0.324 0.281 , 0.323	Depositor DCC
R_{free} test set	2013 reflections (8.33%)	wwPDB-VP
Wilson B-factor (Å^2)	133.2	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 71.2	EDS
L-test for twinning[2]	$< |L| > = 0.31, < L^2 > = 0.14$	Xtriage
Estimated twinning fraction	0.206 for -h,-k,l	Xtriage
F_o,F_c correlation	0.71	EDS
Total number of atoms	16154	wwPDB-VP
Average B, all atoms (Å^2)	173.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: 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	0.26	0/1283	0.47	0/1740
1	C	0.26	0/1242	0.47	0/1686
1	E	0.26	0/1219	0.47	0/1656
2	B	0.26	0/851	0.45	0/1159
2	D	0.25	0/837	0.44	0/1139
2	F	0.25	0/829	0.43	0/1128
3	H	0.24	0/1639	0.47	0/2236
3	M	0.25	0/1666	0.47	0/2271
3	Q	0.26	0/1697	0.48	0/2314
4	L	0.26	0/1631	0.50	0/2218
4	N	0.26	0/1640	0.48	0/2229
4	R	0.26	0/1643	0.48	0/2234
All	All	0.26	0/16177	0.47	0/22010

There are no bond length outliers.

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	1252	0	1229	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1213	0	1194	29	0
1	E	1190	0	1168	25	0
2	B	830	0	806	26	0
2	D	816	0	794	19	0
2	F	809	0	786	27	0
3	H	1598	0	1560	33	0
3	M	1625	0	1588	59	0
3	Q	1655	0	1618	33	0
4	L	1597	0	1537	32	0
4	N	1606	0	1550	33	0
4	R	1608	0	1558	34	0
5	G	38	0	34	3	0
6	I	100	0	85	2	0
6	J	100	0	85	4	0
7	K	89	0	76	1	0
8	C	14	0	13	1	0
8	E	14	0	13	0	0
All	All	16154	0	15694	327	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 10.

The worst 5 of 327 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)
3:M:72:ARG:CG	3:M:79:LEU:HD13	1.62	1.28
3:M:72:ARG:CG	3:M:79:LEU:CD1	2.37	1.01
3:M:29:PHE:CE1	3:M:72:ARG:NH1	2.29	1.00
3:M:72:ARG:HG2	3:M:79:LEU:HD13	1.38	1.00
1:E:162:TYR:HB2	1:E:165:LEU:O	1.66	0.95

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	161/163 (99%)	157 (98%)	4 (2%)	0	100	100
1	C	157/163 (96%)	152 (97%)	5 (3%)	0	100	100
1	E	154/163 (94%)	150 (97%)	4 (3%)	0	100	100
2	B	104/111 (94%)	101 (97%)	3 (3%)	0	100	100
2	D	102/111 (92%)	99 (97%)	3 (3%)	0	100	100
2	F	101/111 (91%)	97 (96%)	4 (4%)	0	100	100
3	H	209/233 (90%)	205 (98%)	4 (2%)	0	100	100
3	M	213/233 (91%)	206 (97%)	7 (3%)	0	100	100
3	Q	220/233 (94%)	215 (98%)	5 (2%)	0	100	100
4	L	206/213 (97%)	200 (97%)	6 (3%)	0	100	100
4	N	207/213 (97%)	204 (99%)	3 (1%)	0	100	100
4	R	209/213 (98%)	204 (98%)	5 (2%)	0	100	100
All	All	2043/2160 (95%)	1990 (97%)	53 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	134/134 (100%)	133 (99%)	1 (1%)	84	90
1	C	130/134 (97%)	130 (100%)	0	100	100
1	E	128/134 (96%)	128 (100%)	0	100	100
2	B	86/90 (96%)	86 (100%)	0	100	100
2	D	85/90 (94%)	85 (100%)	0	100	100
2	F	84/90 (93%)	84 (100%)	0	100	100
3	H	176/194 (91%)	175 (99%)	1 (1%)	86	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	M	180/194 (93%)	178 (99%)	2 (1%)	73	85
3	Q	183/194 (94%)	180 (98%)	3 (2%)	62	79
4	L	184/187 (98%)	183 (100%)	1 (0%)	88	93
4	N	185/187 (99%)	185 (100%)	0	100	100
4	R	185/187 (99%)	182 (98%)	3 (2%)	62	79
All	All	1740/1815 (96%)	1729 (99%)	11 (1%)	86	92

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	M	111	TYR
3	Q	27	PHE
4	R	4	LEU
3	M	27	PHE
3	Q	72	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates (i)

26 monosaccharides 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
5	NAG	G	1	1,5	14,14,15	0.29	0	17,19,21	0.74	0
5	NAG	G	2	5	14,14,15	0.27	0	17,19,21	0.62	0
5	FUC	G	3	5	10,10,11	0.24	0	14,14,16	0.64	0
6	NAG	I	1	2,6	14,14,15	0.35	0	17,19,21	0.45	0
6	NAG	I	2	6	14,14,15	0.30	0	17,19,21	0.49	0
6	BMA	I	3	6	11,11,12	0.43	0	15,15,17	0.88	1 (6%)
6	MAN	I	4	6	11,11,12	1.10	1 (9%)	15,15,17	1.19	2 (13%)
6	NAG	I	5	6	14,14,15	0.24	0	17,19,21	0.55	0
6	GAL	I	6	6	11,11,12	0.57	0	15,15,17	0.97	0
6	MAN	I	7	6	11,11,12	1.05	1 (9%)	15,15,17	1.76	2 (13%)
6	NAG	I	8	6	14,14,15	0.32	0	17,19,21	0.45	0
6	NAG	J	1	2,6	14,14,15	0.34	0	17,19,21	0.42	0
6	NAG	J	2	6	14,14,15	0.26	0	17,19,21	0.47	0
6	BMA	J	3	6	11,11,12	0.54	0	15,15,17	0.92	1 (6%)
6	MAN	J	4	6	11,11,12	0.91	1 (9%)	15,15,17	1.18	2 (13%)
6	NAG	J	5	6	14,14,15	0.28	0	17,19,21	0.50	0
6	GAL	J	6	6	11,11,12	0.51	0	15,15,17	1.00	1 (6%)
6	MAN	J	7	6	11,11,12	1.10	1 (9%)	15,15,17	1.07	0
6	NAG	J	8	6	14,14,15	0.35	0	17,19,21	0.46	0
7	NAG	K	1	2,7	14,14,15	0.40	0	17,19,21	0.45	0
7	NAG	K	2	7	14,14,15	0.29	0	17,19,21	0.51	0
7	BMA	K	3	7	11,11,12	0.73	0	15,15,17	0.90	1 (6%)
7	MAN	K	4	7	11,11,12	0.79	0	15,15,17	1.23	2 (13%)
7	NAG	K	5	7	14,14,15	0.33	0	17,19,21	0.70	0
7	MAN	K	6	7	11,11,12	0.94	1 (9%)	15,15,17	1.10	2 (13%)
7	NAG	K	7	7	14,14,15	0.34	0	17,19,21	0.52	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
5	NAG	G	1	1,5	-	5/6/23/26	0/1/1/1
5	NAG	G	2	5	-	3/6/23/26	0/1/1/1
5	FUC	G	3	5	-	-	0/1/1/1
6	NAG	I	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	3/6/23/26	0/1/1/1
6	BMA	I	3	6	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	I	4	6	-	0/2/19/22	0/1/1/1
6	NAG	I	5	6	-	0/6/23/26	0/1/1/1
6	GAL	I	6	6	-	1/2/19/22	0/1/1/1
6	MAN	I	7	6	-	2/2/19/22	0/1/1/1
6	NAG	I	8	6	-	1/6/23/26	0/1/1/1
6	NAG	J	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	J	2	6	-	1/6/23/26	0/1/1/1
6	BMA	J	3	6	-	2/2/19/22	0/1/1/1
6	MAN	J	4	6	-	0/2/19/22	0/1/1/1
6	NAG	J	5	6	-	1/6/23/26	0/1/1/1
6	GAL	J	6	6	-	1/2/19/22	0/1/1/1
6	MAN	J	7	6	-	1/2/19/22	0/1/1/1
6	NAG	J	8	6	-	3/6/23/26	0/1/1/1
7	NAG	K	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	K	2	7	-	1/6/23/26	0/1/1/1
7	BMA	K	3	7	-	2/2/19/22	0/1/1/1
7	MAN	K	4	7	-	1/2/19/22	0/1/1/1
7	NAG	K	5	7	-	3/6/23/26	0/1/1/1
7	MAN	K	6	7	-	0/2/19/22	0/1/1/1
7	NAG	K	7	7	-	1/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	4	MAN	C1-C2	2.70	1.58	1.52
7	K	6	MAN	C1-C2	2.58	1.58	1.52
6	J	4	MAN	C1-C2	2.52	1.58	1.52
6	I	7	MAN	O5-C5	2.47	1.48	1.43
6	J	7	MAN	C2-C3	2.43	1.56	1.52

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	7	MAN	C1-O5-C5	5.94	120.23	112.19
7	K	4	MAN	C1-O5-C5	3.13	116.43	112.19
6	J	4	MAN	O2-C2-C3	-2.80	104.53	110.14
6	I	4	MAN	O2-C2-C1	2.68	114.63	109.15
7	K	4	MAN	O2-C2-C3	-2.44	105.24	110.14

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	1	NAG	C8-C7-N2-C2
5	G	1	NAG	O7-C7-N2-C2
5	G	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
6	I	3	BMA	C4-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	8	NAG	2	0
7	K	3	BMA	1	0
6	J	5	NAG	1	0
6	I	1	NAG	1	0
6	J	3	BMA	1	0
6	I	8	NAG	1	0
5	G	2	NAG	3	0
7	K	6	MAN	1	0

5.6 Ligand geometry (i)

2 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	$\#|Z| > 2$
8	NAG	E	300	1	14,14,15	0.24	0	17,19,21	0.49	0
8	NAG	C	300	1	14,14,15	0.38	0	17,19,21	1.23	1 (5%)

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
8	NAG	E	300	1	-	2/6/23/26	0/1/1/1
8	NAG	C	300	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	300	NAG	C2-N2-C7	4.29	129.01	122.90

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	300	NAG	C8-C7-N2-C2
8	C	300	NAG	O7-C7-N2-C2
8	E	300	NAG	O5-C5-C6-O6
8	C	300	NAG	O5-C5-C6-O6
8	E	300	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	300	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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.