



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 06:33 pm GMT

PDB ID : 5JS9
Title : Uncleaved prefusion optimized gp140 trimer with an engineered 8-residue HR1 turn bound to broadly neutralizing antibodies 8ANC195 and PGT128
Authors : Kong, L.; Wilson, I.A.
Deposited on : 2016-05-07
Resolution : 6.92 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

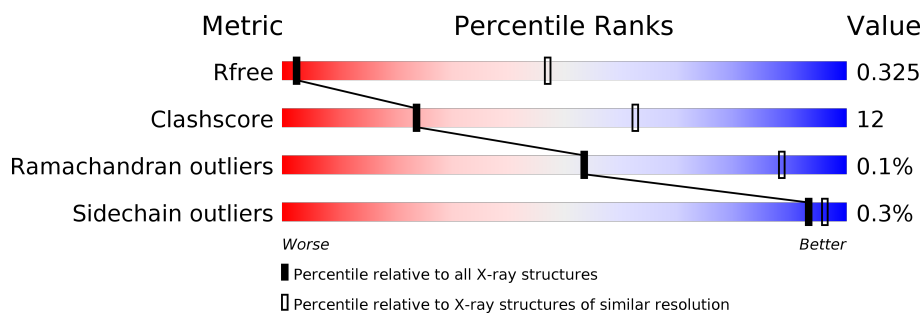
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.92 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}	111664	1067 (10.00-3.80)
Clashscore	122126	1146 (10.00-3.80)
Ramachandran outliers	120053	1071 (10.00-3.80)
Sidechain outliers	120020	1038 (10.00-3.80)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	239	<div> <div>75%</div> <div>21%</div> <div>.</div> </div>
2	B	211	<div> <div>71%</div> <div>26%</div> <div>.</div> </div>
3	C	480	<div> <div>68%</div> <div>25%</div> <div>7%</div> </div>
4	D	140	<div> <div>66%</div> <div>26%</div> <div>.</div> <div>7%</div> </div>
5	E	238	<div> <div>69%</div> <div>25%</div> <div>6%</div> </div>
6	F	215	<div> <div>74%</div> <div>25%</div> <div>.</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	MAN	C	666	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12007 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 broadly neutralizing antibody PGT128 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1735	1105	292	332	6			

- Molecule 2 is a protein called broadly neutralizing antibody PGT128 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	204	Total	C	N	O	S	0	0	0
			1514	950	254	306	4			

- Molecule 3 is a protein called gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	447	Total	C	N	O	S	0	0	0
			3519	2210	622	659	28			

- Molecule 4 is a protein called gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	130	Total	C	N	O	S	0	0	0
			1039	655	178	199	7			

- Molecule 5 is a protein called broadly neutralizing antibody 8ANC195 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	224	Total	C	N	O	S	0	0	0
			1686	1072	284	325	5			

- Molecule 6 is a protein called broadly neutralizing antibody 8ANC195 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	212	Total	C	N	O	S	0	0	0
			1626	1018	279	324	5			

- Molecule 7 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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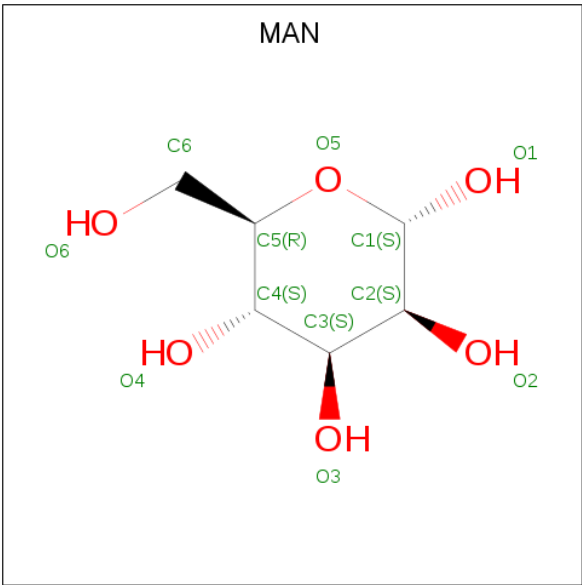
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1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

- Molecule 8 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 9 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		

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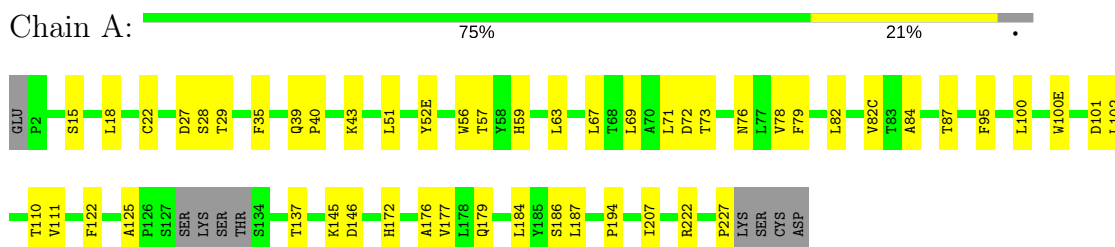
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	D	1	Total	C	O	0	0
			11	6	5		

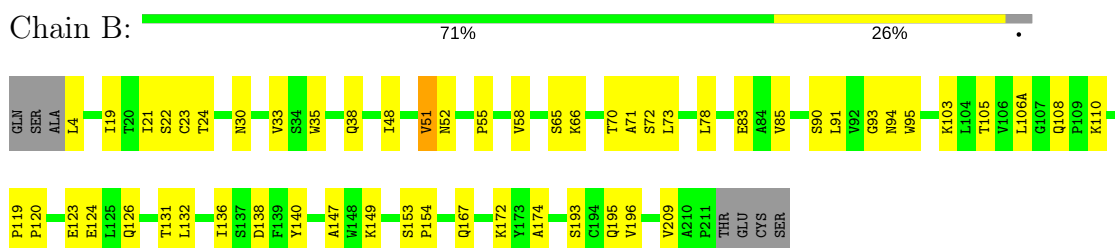
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

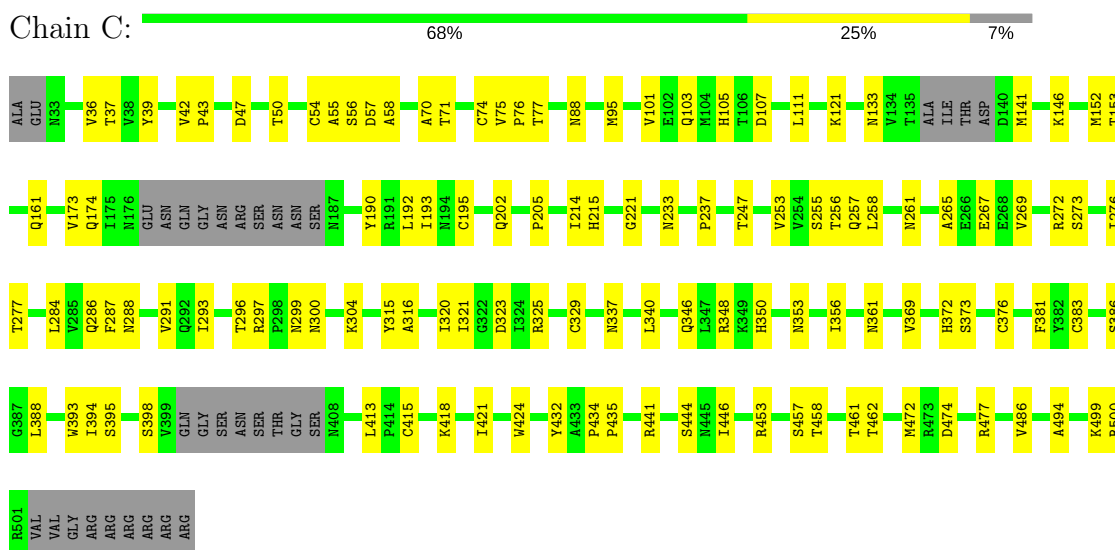
- Molecule 1: broadly neutralizing antibody PGT128 heavy chain



- Molecule 2: broadly neutralizing antibody PGT128 light chain



- Molecule 3: gp120



- Molecule 4: gp41

L633	E634	ALA
E635	GLY	VAL
S636	ILE	GLY
Q637	GLY	ILE
M638	ALA	ALA
Q639	VAL	PHE
E641	LEU	GLY
L647	F622	
L650	G527	
D651	Q640	
	L544	
	M548	
	P549	
	D550	
	M551	
	F552	
	P553	
	V557	
	M558	
	K561	
	L580	
	M583	
	K588	
	C592	
	T593	
	M594	
	V595	
	F596	
	M597	
	N598	
	M601	
	S602	
	M603	
	R604	
	M605	
	E608	
	M618	
	D619	
	K620	
	E621	
	I622	
	S623	
	L632	

- Chain E: 69% 25% 6%

CYS		V130		G1
ASP		T135		T2
LYS		P138		H3
THR		P145		L4
		S146		K12
		S147		S17
		LYS		V18
		SER		T19
		THR		A24
		SER		Y25
		GLY		F30
		G153		A34
		L157		R39
		G158		Q40
		K162		A41
		D163		O44
		Y164		S45
		P166		L46
		S172		I49
		W173		W53
		L178		R54
		A187		W55
		L194		A59
		L197		S60
		V201		H61
		S205		R64
		SER		G65
		SER		R66
		LEU		V67
		GLY		D73
		T210		L74
		Q211		T75
		T212		S78
		T213		P79
		T214		L84
		C215		E85
		N216		T94
		H219		T101
		K220		G110
		P221		G121
		K229		S121
		K233		W122
		SER		C122

- Chain F: 74% 25%

N137	M138	F139	Y140	P141	R142	Q160	S162	V163		Q166	D170	S171	T172	Y173	S174	L175	S176	S177	T178	L179	H189	V196	N210	R211	GLY	GLU	CYS		D1	M4	S12	G16	V19	S22	I29	T30	W32	Q37	Q38	L47	B50	P59	S60	R61	S65	F71	T72	I75	G76	N77	F83	Y91	Y94	P95	G99	E105	V106	K107	R108	P113	S114	V115	Q124	S131	T136
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4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	261.95Å 261.95Å 261.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.83 – 6.92 47.83 – 6.92	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.83-6.92) 91.0 (47.83-6.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 6.68Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.284 , 0.322 0.291 , 0.325	Depositor DCC
R_{free} test set	493 reflections (9.82%)	wwPDB-VP
Wilson B-factor (Å ²)	334.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 230.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.067 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	12007	wwPDB-VP
Average B, all atoms (Å ²)	291.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, 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	0.21	0/1786	0.41	0/2449
2	B	0.22	0/1552	0.47	1/2121 (0.0%)
3	C	0.23	0/3592	0.44	0/4875
4	D	0.26	0/1061	0.51	0/1444
5	E	0.23	0/1730	0.44	0/2361
6	F	0.24	0/1661	0.44	0/2256
All	All	0.23	0/11382	0.45	1/15506 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	108	GLN	C-N-CD	-9.05	100.68	120.60

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	1735	0	1690	33	0
2	B	1514	0	1473	41	0
3	C	3519	0	3460	101	0
4	D	1039	0	1003	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1686	0	1659	55	0
6	F	1626	0	1581	41	0
7	C	406	0	355	14	0
7	D	42	0	37	2	0
8	C	99	0	79	0	0
8	D	11	0	9	1	0
9	C	319	0	272	17	0
9	D	11	0	10	0	0
All	All	12007	0	11628	283	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 12.

The worst 5 of 283 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:C:76:PRO:HD2	4:D:551:TRP:CE2	1.53	1.42
3:C:76:PRO:HG2	4:D:551:TRP:CZ2	1.53	1.41
3:C:76:PRO:HD2	4:D:551:TRP:NE1	1.44	1.31
3:C:76:PRO:CG	4:D:551:TRP:CZ2	2.26	1.18
3:C:76:PRO:HG2	4:D:551:TRP:CH2	1.80	1.15

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	226/239 (95%)	212 (94%)	14 (6%)	0	100	100
2	B	202/211 (96%)	193 (96%)	8 (4%)	1 (0%)	31	74
3	C	439/480 (92%)	417 (95%)	22 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	128/140 (91%)	118 (92%)	10 (8%)	0	100	100
5	E	218/238 (92%)	209 (96%)	9 (4%)	0	100	100
6	F	210/215 (98%)	205 (98%)	5 (2%)	0	100	100
All	All	1423/1523 (93%)	1354 (95%)	68 (5%)	1 (0%)	53	88

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL

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	194/203 (96%)	194 (100%)	0	100	100
2	B	171/177 (97%)	171 (100%)	0	100	100
3	C	399/426 (94%)	397 (100%)	2 (0%)	90	95
4	D	113/118 (96%)	112 (99%)	1 (1%)	81	90
5	E	192/204 (94%)	191 (100%)	1 (0%)	90	95
6	F	180/182 (99%)	180 (100%)	0	100	100
All	All	1249/1310 (95%)	1245 (100%)	4 (0%)	93	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	233	ASN
3	C	337	ASN
4	D	548	ASN
5	E	64	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
5	E	40	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

72 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	$\# Z > 2$
7	NAG	C	601	3,7	14,14,15	0.29	0	17,19,21	0.69	0
7	NAG	C	602	7	14,14,15	0.19	0	17,19,21	0.43	0
7	NAG	C	603	3	14,14,15	0.28	0	17,19,21	0.47	0
7	NAG	C	604	3,7	14,14,15	0.21	0	17,19,21	0.47	0
7	NAG	C	605	7	14,14,15	0.27	0	17,19,21	0.46	0
7	NAG	C	606	3	14,14,15	0.34	0	17,19,21	0.58	0
7	NAG	C	607	3,7	14,14,15	0.21	0	17,19,21	1.03	1 (5%)
7	NAG	C	608	7	14,14,15	0.24	0	17,19,21	0.42	0
7	NAG	C	609	3,7	14,14,15	0.28	0	17,19,21	0.55	0
7	NAG	C	610	7	14,14,15	0.26	0	17,19,21	0.42	0
7	NAG	C	611	3,7	14,14,15	0.60	0	17,19,21	0.56	0
7	NAG	C	612	8,7	14,14,15	0.56	0	17,19,21	0.51	0
8	BMA	C	613	9,7	11,11,12	0.55	0	15,15,17	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	MAN	C	614	9,8	11,11,12	0.67	0	15,15,17	1.07	1 (6%)
9	MAN	C	615	9	11,11,12	0.57	0	15,15,17	1.04	1 (6%)
9	MAN	C	616	9,8	11,11,12	0.89	0	15,15,17	0.92	2 (13%)
9	MAN	C	617	9	11,11,12	0.79	1 (9%)	15,15,17	1.47	2 (13%)
9	MAN	C	618	9	11,11,12	0.63	0	15,15,17	1.03	2 (13%)
7	NAG	C	619	3	14,14,15	0.36	0	17,19,21	0.41	0
7	NAG	C	620	3,7	14,14,15	0.25	0	17,19,21	0.48	0
7	NAG	C	621	8,7	14,14,15	0.22	0	17,19,21	0.44	0
9	MAN	C	622	9	11,11,12	0.66	0	15,15,17	1.25	2 (13%)
9	MAN	C	623	9	11,11,12	0.67	0	15,15,17	0.93	1 (6%)
8	BMA	C	624	9,7	11,11,12	0.79	0	15,15,17	0.88	0
9	MAN	C	625	9,8	11,11,12	0.75	1 (9%)	15,15,17	1.15	2 (13%)
9	MAN	C	626	9,8	11,11,12	0.68	0	15,15,17	1.05	2 (13%)
9	MAN	C	627	9	11,11,12	0.68	0	15,15,17	1.00	2 (13%)
9	MAN	C	628	9	11,11,12	0.68	0	15,15,17	1.15	2 (13%)
9	MAN	C	629	9	11,11,12	0.80	0	15,15,17	0.97	1 (6%)
7	NAG	C	630	3,7	14,14,15	0.48	0	17,19,21	0.66	0
7	NAG	C	631	8,7	14,14,15	0.20	0	17,19,21	0.72	0
8	BMA	C	632	9,7	11,11,12	0.80	0	15,15,17	1.03	0
9	MAN	C	633	9,8	11,11,12	0.70	0	15,15,17	0.99	2 (13%)
9	MAN	C	634	9	11,11,12	0.66	0	15,15,17	0.99	2 (13%)
9	MAN	C	635	9,8	11,11,12	0.78	0	15,15,17	1.34	2 (13%)
9	MAN	C	636	9	11,11,12	0.60	0	15,15,17	1.14	2 (13%)
9	MAN	C	637	9	11,11,12	0.58	0	15,15,17	1.14	2 (13%)
7	NAG	C	638	3,7	14,14,15	0.30	0	17,19,21	0.50	0
7	NAG	C	639	8,7	14,14,15	0.43	0	17,19,21	0.56	0
8	BMA	C	640	9,7	11,11,12	0.65	0	15,15,17	1.02	1 (6%)
9	MAN	C	641	8	11,11,12	0.76	1 (9%)	15,15,17	1.17	2 (13%)
9	MAN	C	642	8	11,11,12	0.70	0	15,15,17	1.33	1 (6%)
7	NAG	C	643	3,7	14,14,15	0.44	0	17,19,21	0.50	0
7	NAG	C	644	8,7	14,14,15	0.23	0	17,19,21	0.65	0
8	BMA	C	645	9,7	11,11,12	0.66	0	15,15,17	1.23	1 (6%)
9	MAN	C	646	9,8	11,11,12	0.61	0	15,15,17	1.33	2 (13%)
9	MAN	C	647	9	11,11,12	0.22	0	15,15,17	0.59	0
7	NAG	C	648	3,7	14,14,15	0.40	0	17,19,21	0.46	0
7	NAG	C	649	8,7	14,14,15	0.27	0	17,19,21	0.64	0
8	BMA	C	650	7	11,11,12	0.63	0	15,15,17	0.79	0
7	NAG	C	651	3,7	14,14,15	0.33	0	17,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	C	652	8,7	14,14,15	0.39	0	17,19,21	0.64	0
8	BMA	C	653	7	11,11,12	0.67	0	15,15,17	0.81	0
7	NAG	C	654	3,7	14,14,15	0.32	0	17,19,21	0.79	0
7	NAG	C	655	8,7	14,14,15	0.23	0	17,19,21	0.69	1 (5%)
8	BMA	C	656	7	11,11,12	0.64	0	15,15,17	0.76	0
7	NAG	C	657	3,7	14,14,15	0.17	0	17,19,21	0.43	0
7	NAG	C	658	8,7	14,14,15	0.38	0	17,19,21	0.49	0
8	BMA	C	659	9,7	11,11,12	0.52	0	15,15,17	0.71	0
9	MAN	C	660	9,8	11,11,12	0.52	0	15,15,17	1.12	2 (13%)
9	MAN	C	661	9	11,11,12	0.71	0	15,15,17	1.07	0
9	MAN	C	662	9	11,11,12	0.52	0	15,15,17	1.01	2 (13%)
9	MAN	C	663	9,8	11,11,12	0.57	0	15,15,17	1.18	2 (13%)
9	MAN	C	664	9	11,11,12	0.63	0	15,15,17	1.19	2 (13%)
9	MAN	C	665	9	11,11,12	0.83	0	15,15,17	1.43	3 (20%)
9	MAN	C	666	9	11,11,12	0.64	0	15,15,17	0.96	2 (13%)
9	MAN	C	667	9	11,11,12	0.58	0	15,15,17	1.04	2 (13%)
7	NAG	D	701	4,7	14,14,15	0.25	0	17,19,21	0.46	0
7	NAG	D	702	8,7	14,14,15	0.42	0	17,19,21	1.51	3 (17%)
8	BMA	D	703	9,7	11,11,12	0.75	0	15,15,17	0.98	0
9	MAN	D	704	8	11,11,12	1.54	3 (27%)	15,15,17	1.38	2 (13%)
7	NAG	D	705	4	14,14,15	0.21	0	17,19,21	0.45	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
7	NAG	C	601	3,7	-	1/6/23/26	0/1/1/1
7	NAG	C	602	7	-	0/6/23/26	0/1/1/1
7	NAG	C	603	3	-	0/6/23/26	0/1/1/1
7	NAG	C	604	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	605	7	-	0/6/23/26	0/1/1/1
7	NAG	C	606	3	-	0/6/23/26	0/1/1/1
7	NAG	C	607	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	608	7	-	0/6/23/26	0/1/1/1
7	NAG	C	609	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	610	7	-	0/6/23/26	0/1/1/1
7	NAG	C	611	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	612	8,7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BMA	C	613	9,7	-	0/2/19/22	0/1/1/1
9	MAN	C	614	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	615	9	-	0/2/19/22	0/1/1/1
9	MAN	C	616	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	617	9	-	0/2/19/22	0/1/1/1
9	MAN	C	618	9	-	0/2/19/22	0/1/1/1
7	NAG	C	619	3	-	0/6/23/26	0/1/1/1
7	NAG	C	620	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	621	8,7	-	0/6/23/26	0/1/1/1
9	MAN	C	622	9	-	0/2/19/22	0/1/1/1
9	MAN	C	623	9	-	0/2/19/22	0/1/1/1
8	BMA	C	624	9,7	-	0/2/19/22	0/1/1/1
9	MAN	C	625	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	626	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	627	9	-	0/2/19/22	0/1/1/1
9	MAN	C	628	9	-	0/2/19/22	0/1/1/1
9	MAN	C	629	9	-	0/2/19/22	0/1/1/1
7	NAG	C	630	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	631	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	632	9,7	-	0/2/19/22	0/1/1/1
9	MAN	C	633	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	634	9	-	0/2/19/22	0/1/1/1
9	MAN	C	635	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	636	9	-	0/2/19/22	0/1/1/1
9	MAN	C	637	9	-	0/2/19/22	0/1/1/1
7	NAG	C	638	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	639	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	640	9,7	-	0/2/19/22	0/1/1/1
9	MAN	C	641	8	-	0/2/19/22	0/1/1/1
9	MAN	C	642	8	-	0/2/19/22	0/1/1/1
7	NAG	C	643	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	644	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	645	9,7	-	0/2/19/22	0/1/1/1
9	MAN	C	646	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	647	9	-	0/2/19/22	0/1/1/1
7	NAG	C	648	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	649	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	650	7	-	0/2/19/22	0/1/1/1
7	NAG	C	651	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	652	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	653	7	-	0/2/19/22	0/1/1/1
7	NAG	C	654	3,7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	C	655	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	656	7	-	0/2/19/22	0/1/1/1
7	NAG	C	657	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	658	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	659	9,7	-	0/2/19/22	0/1/1/1
9	MAN	C	660	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	661	9	-	0/2/19/22	0/1/1/1
9	MAN	C	662	9	-	0/2/19/22	0/1/1/1
9	MAN	C	663	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	664	9	-	0/2/19/22	0/1/1/1
9	MAN	C	665	9	-	0/2/19/22	0/1/1/1
9	MAN	C	666	9	-	0/2/19/22	0/1/1/1
9	MAN	C	667	9	-	0/2/19/22	0/1/1/1
7	NAG	D	701	4,7	-	0/6/23/26	0/1/1/1
7	NAG	D	702	8,7	-	0/6/23/26	0/1/1/1
8	BMA	D	703	9,7	-	0/2/19/22	0/1/1/1
9	MAN	D	704	8	-	0/2/19/22	0/1/1/1
7	NAG	D	705	4	-	0/6/23/26	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	625	MAN	C1-C2	2.09	1.57	1.52
9	C	617	MAN	C1-C2	2.16	1.57	1.52
9	C	641	MAN	C1-C2	2.26	1.57	1.52
9	D	704	MAN	C1-C2	2.56	1.58	1.52
9	D	704	MAN	O2-C2	2.68	1.49	1.43

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	665	MAN	O2-C2-C3	-3.42	103.52	110.19
9	C	628	MAN	O2-C2-C3	-3.23	103.89	110.19
9	C	622	MAN	O2-C2-C3	-3.11	104.12	110.19
8	C	640	BMA	C1-C2-C3	-2.75	106.18	109.66
9	C	667	MAN	O2-C2-C3	-2.56	105.21	110.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	601	NAG	O7-C7-N2-C2

There are no ring outliers.

19 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	601	NAG	2	0
7	C	606	NAG	1	0
7	C	608	NAG	1	0
7	C	609	NAG	2	0
7	C	610	NAG	1	0
7	C	612	NAG	2	0
9	C	623	MAN	1	0
9	C	628	MAN	2	0
9	C	629	MAN	3	0
7	C	638	NAG	3	0
7	C	639	NAG	2	0
7	C	649	NAG	1	0
7	C	654	NAG	1	0
7	C	657	NAG	1	0
7	C	658	NAG	2	0
9	C	662	MAN	3	0
9	C	666	MAN	8	0
7	D	702	NAG	2	0
8	D	703	BMA	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 ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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