



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 14, 2017 – 01:18 AM EST

PDB ID : 5UTY
Title : Crystal Structure of a Stabilized DS-SOSIP.mut4 BG505 gp140 HIV-1 Env Trimer, Containing Mutations I201C-P433C (DS), L154M, N300M, N302M, T320L in Complex with Human Antibodies PGT122 and 35O22 at 4.1 Angstrom
Authors : Xu, K.; Chuang, G.-Y.; Pancera, M.; Kwong, P.D.
Deposited on : unknown
Resolution : 3.41 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

<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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

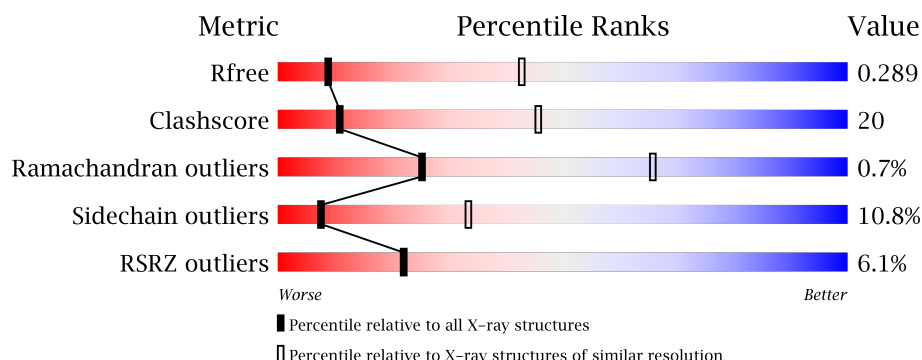
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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}	100719	1074 (3.50-3.34)
Clashscore	112137	1179 (3.50-3.34)
Ramachandran outliers	110173	1147 (3.50-3.34)
Sidechain outliers	110143	1148 (3.50-3.34)
RSRZ outliers	101464	1100 (3.50-3.34)

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	B	153	<div> <div>20%</div> <div>47% 25% 7% 20%</div> </div>
2	D	243	<div> <div>15%</div> <div>57% 39%</div> </div>
3	E	216	<div> <div>15%</div> <div>68% 28%</div> </div>
4	G	505	<div> <div>53% 28% 8% 11%</div> </div>
5	H	235	<div> <div>66% 29%</div> </div>

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Mol	Chain	Length	Quality of chain
6	L	208	 <div>63% 35%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	NAG	G	634	-	-	X	-
7	NAG	G	635	-	-	X	-
9	MAN	G	641	-	-	X	-
9	MAN	G	642	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 12020 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 HIV-1 BG505 strain Env gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	122	Total	C	N	O	S	0	0	0
			969	611	168	184	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S6
B	605	CYS	THR	engineered mutation	UNP Q2N0S6

- Molecule 2 is a protein called 35O22 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	242	Total	C	N	O	S	0	0	0
			1820	1156	303	353	8			

- Molecule 3 is a protein called 35O22 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	213	Total	C	N	O	S	0	0	0
			1615	1012	267	328	8			

- Molecule 4 is a protein called HIV-1 BG505 strain Env gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	449	Total	C	N	O	S	0	0	0
			3542	2224	623	662	33			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	7	MET	-	initiating methionine	UNP Q2N0S6
G	8	PRO	-	expression tag	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	9	MET	-	expression tag	UNP Q2N0S6
G	10	GLY	-	expression tag	UNP Q2N0S6
G	11	SER	-	expression tag	UNP Q2N0S6
G	12	LEU	-	expression tag	UNP Q2N0S6
G	13	GLN	-	expression tag	UNP Q2N0S6
G	14	PRO	-	expression tag	UNP Q2N0S6
G	15	LEU	-	expression tag	UNP Q2N0S6
G	16	ALA	-	expression tag	UNP Q2N0S6
G	17	THR	-	expression tag	UNP Q2N0S6
G	18	LEU	-	expression tag	UNP Q2N0S6
G	19	TYR	-	expression tag	UNP Q2N0S6
G	20	LEU	-	expression tag	UNP Q2N0S6
G	21	LEU	-	expression tag	UNP Q2N0S6
G	22	GLY	-	expression tag	UNP Q2N0S6
G	23	MET	-	expression tag	UNP Q2N0S6
G	24	LEU	-	expression tag	UNP Q2N0S6
G	25	VAL	-	expression tag	UNP Q2N0S6
G	26	ALA	-	expression tag	UNP Q2N0S6
G	27	SER	-	expression tag	UNP Q2N0S6
G	28	VAL	-	expression tag	UNP Q2N0S6
G	29	LEU	-	expression tag	UNP Q2N0S6
G	154	MET	LEU	engineered mutation	UNP Q2N0S6
G	201	CYS	ILE	engineered mutation	UNP Q2N0S6
G	300	MET	ASN	engineered mutation	UNP Q2N0S6
G	302	MET	ASN	engineered mutation	UNP Q2N0S6
G	320	LEU	THR	engineered mutation	UNP Q2N0S6
G	332	ASN	THR	engineered mutation	UNP Q2N0S6
G	433	CYS	ALA	engineered mutation	UNP Q2N0S6
G	501	CYS	ALA	engineered mutation	UNP Q2N0S6
G	509	ARG	-	insertion	UNP Q2N0S6
G	510	ARG	-	insertion	UNP Q2N0S6
G	511	ARG	-	insertion	UNP Q2N0S6
G	512	ARG	-	insertion	UNP Q2N0S6
G	513	ARG	-	insertion	UNP Q2N0S6

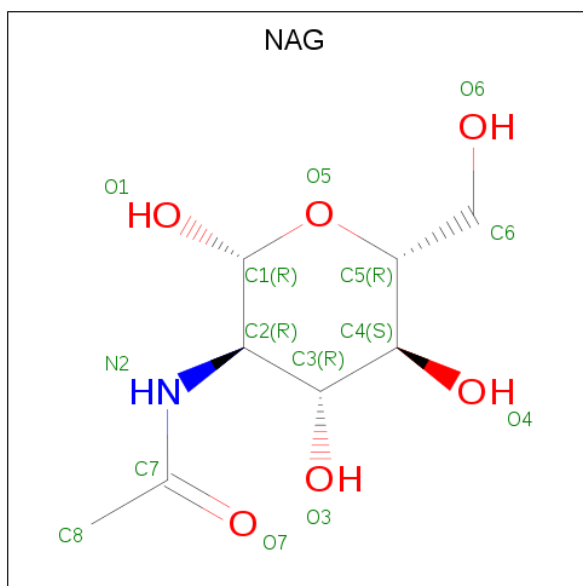
- Molecule 5 is a protein called PGT122 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	232	Total	C	N	O	S	0	0	0
			1762	1121	299	337	5			

- Molecule 6 is a protein called PGT122 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	208	Total	C	N	O	S	0	0	0
			1577	990	265	318	4			

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



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

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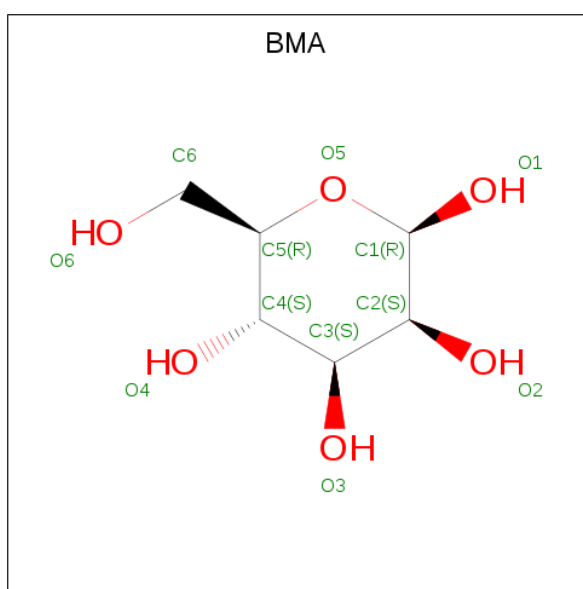
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1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

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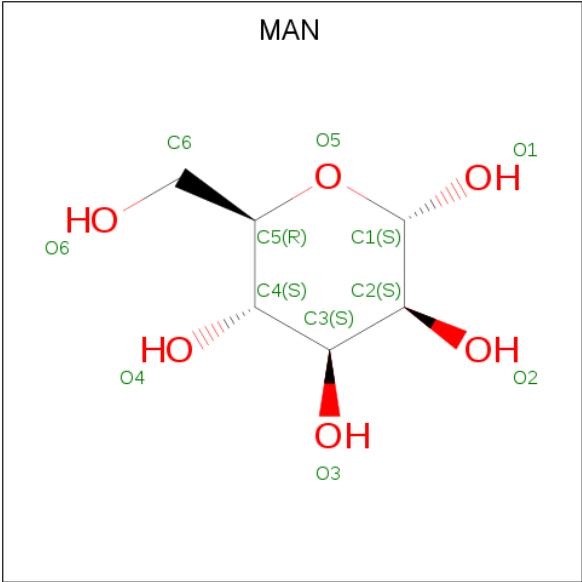
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	H	1	Total	C	N	O	0	0
			14	8	1	5		

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



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

- Molecule 9 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



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

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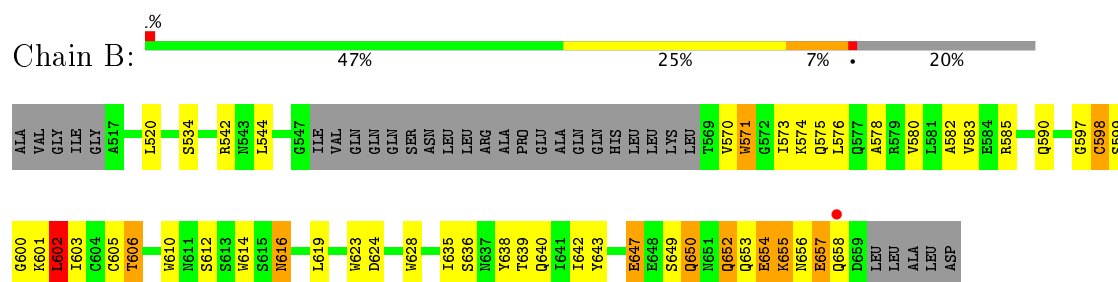
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		

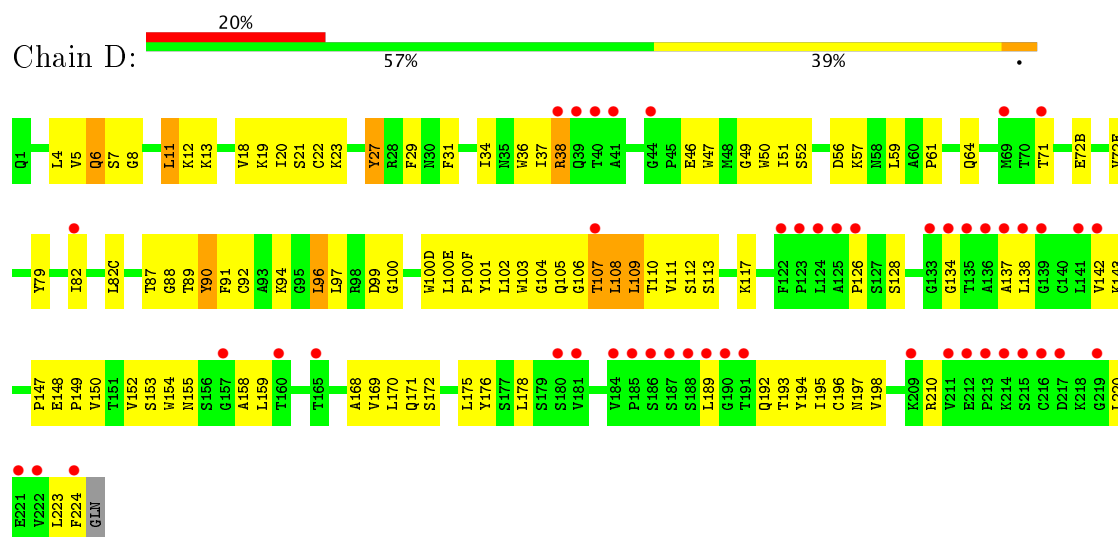
3 Residue-property plots [i](#)

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 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.

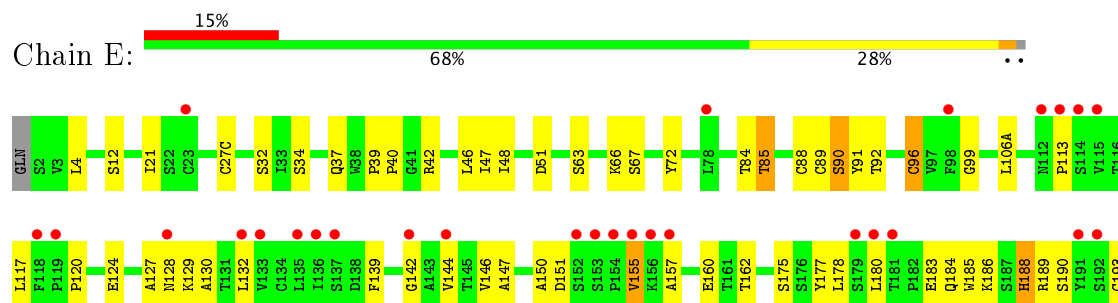
- Molecule 1: HIV-1 BG505 strain Env gp41

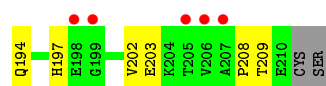


- Molecule 2: 35O22 Fab heavy chain

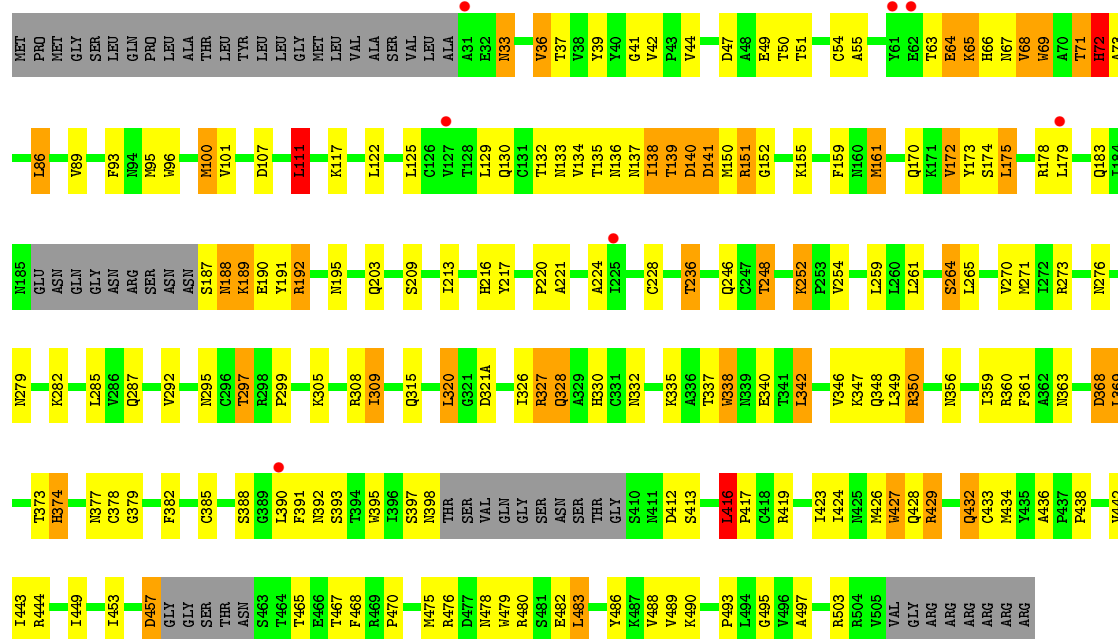


- Molecule 3: 35O22 Fab light chain

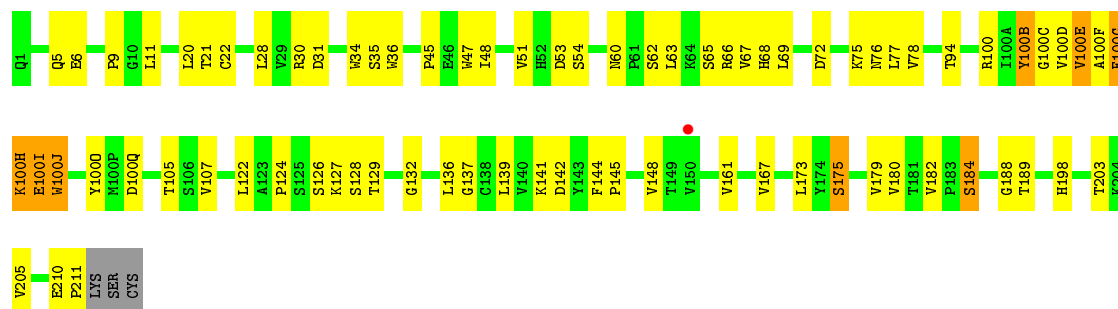




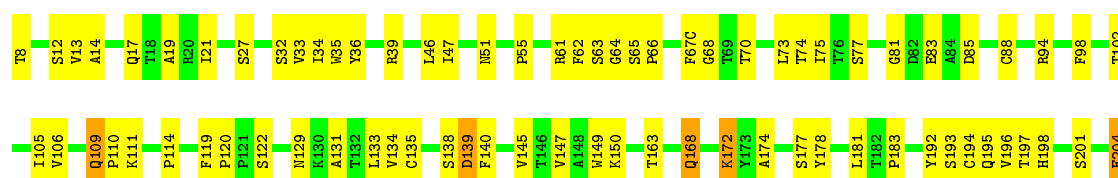
• Molecule 4: HIV-1 BG505 strain Env gp120



• Molecule 5: PGT122 Fab heavy chain



• Molecule 6: PGT122 Fab light chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	131.45Å 131.45Å 312.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.48 – 3.41 41.48 – 3.41	Depositor EDS
% Data completeness (in resolution range)	58.0 (41.48-3.41) 58.0 (41.48-3.41)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.241 , 0.288 0.241 , 0.289	Depositor DCC
R_{free} test set	1270 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	86.6	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 31.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.138 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	12020	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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 [i](#)

5.1 Standard geometry [i](#)

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	B	0.46	0/987	0.62	1/1338 (0.1%)
2	D	0.29	0/1867	0.55	1/2544 (0.0%)
3	E	0.25	0/1659	0.47	0/2269
4	G	0.35	0/3615	0.62	2/4903 (0.0%)
5	H	0.50	2/1810 (0.1%)	0.53	0/2474
6	L	0.25	0/1619	0.49	0/2217
All	All	0.36	2/11557 (0.0%)	0.56	4/15745 (0.0%)

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
4	G	0	1
5	H	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	100(I)	GLU	CD-OE1	-10.57	1.14	1.25
5	H	100(I)	GLU	CD-OE2	8.65	1.35	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	416	LEU	C-N-CD	-19.82	77.00	120.60
2	D	96	LEU	CA-CB-CG	5.93	128.95	115.30
1	B	600	GLY	N-CA-C	-5.30	99.84	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	111	LEU	CA-CB-CG	5.20	127.26	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	G	416	LEU	Mainchain
5	H	100(G)	PHE	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	B	969	0	938	42	2
2	D	1820	0	1788	127	0
3	E	1615	0	1542	43	0
4	G	3542	0	3475	140	0
5	H	1762	0	1724	81	0
6	L	1577	0	1518	51	0
7	B	42	0	39	0	0
7	G	448	0	397	32	0
7	H	14	0	13	1	0
8	G	55	0	41	2	0
9	G	176	0	153	13	0
All	All	12020	0	11628	480	2

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 20.

The worst 5 of 480 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)
2:D:109:LEU:HD12	2:D:110:THR:N	1.29	1.48
7:G:635:NAG:H2	5:H:100(D):VAL:HA	1.29	1.11
2:D:8:GLY:HA2	2:D:107:THR:HG23	1.19	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:7:SER:O	2:D:107:THR:HG21	1.52	1.10
1:B:590:GLN:HE22	1:B:601:LYS:HE2	1.09	1.09

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:ARG:CZ	1:B:647:GLU:OE2[3_845]	1.87	0.33
1:B:542:ARG:NE	1:B:647:GLU:OE2[3_845]	1.93	0.27

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	B	118/153 (77%)	109 (92%)	7 (6%)	2 (2%)	11	48
2	D	240/243 (99%)	230 (96%)	10 (4%)	0	100	100
3	E	211/216 (98%)	206 (98%)	5 (2%)	0	100	100
4	G	441/505 (87%)	404 (92%)	32 (7%)	5 (1%)	17	57
5	H	230/235 (98%)	214 (93%)	13 (6%)	3 (1%)	14	53
6	L	206/208 (99%)	190 (92%)	16 (8%)	0	100	100
All	All	1446/1560 (93%)	1353 (94%)	83 (6%)	10 (1%)	25	66

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	G	72	HIS
5	H	100(E)	VAL
1	B	602	LEU
4	G	328	GLN
4	G	417	PRO

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	B	104/129 (81%)	83 (80%)	21 (20%)	1	6
2	D	203/206 (98%)	190 (94%)	13 (6%)	20	58
3	E	186/189 (98%)	175 (94%)	11 (6%)	23	61
4	G	403/448 (90%)	333 (83%)	70 (17%)	2	12
5	H	198/205 (97%)	188 (95%)	10 (5%)	28	64
6	L	177/177 (100%)	165 (93%)	12 (7%)	18	56
All	All	1271/1354 (94%)	1134 (89%)	137 (11%)	7	33

5 of 137 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	G	132	THR
4	G	213	ILE
6	L	67(C)	PHE
4	G	134	VAL
4	G	161	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	590	GLN
1	B	652	GLN
2	D	6	GLN
4	G	130	GLN
4	G	188	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

57 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	B	701	1	14,14,15	0.48	0	15,19,21	0.47	0
7	NAG	B	702	1	14,14,15	0.23	0	15,19,21	0.56	0
7	NAG	B	703	1	14,14,15	0.26	0	15,19,21	0.53	0
7	NAG	G	601	4,7	14,14,15	0.38	0	15,19,21	0.48	0
7	NAG	G	602	8,7	14,14,15	0.45	0	15,19,21	1.26	1 (6%)
8	BMA	G	603	9,7	11,11,12	1.12	1 (9%)	13,15,17	0.96	1 (7%)
9	MAN	G	604	8	11,11,12	0.76	1 (9%)	13,15,17	1.30	2 (15%)
9	MAN	G	605	9,8	11,11,12	1.35	1 (9%)	13,15,17	1.74	3 (23%)
9	MAN	G	606	9	11,11,12	1.15	1 (9%)	13,15,17	1.79	3 (23%)
7	NAG	G	607	4	14,14,15	0.54	0	15,19,21	0.54	0
7	NAG	G	608	4,7	14,14,15	0.40	0	15,19,21	0.48	0
7	NAG	G	609	8,7	14,14,15	0.29	0	15,19,21	0.46	0
8	BMA	G	610	9,7	11,11,12	0.56	0	13,15,17	0.80	0
9	MAN	G	611	8	11,11,12	0.93	1 (9%)	13,15,17	1.38	2 (15%)
7	NAG	G	612	4,7	14,14,15	0.30	0	15,19,21	0.48	0
7	NAG	G	613	8,7	14,14,15	0.18	0	15,19,21	0.45	0
8	BMA	G	614	9,7	11,11,12	0.56	0	13,15,17	0.68	0
9	MAN	G	615	8	11,11,12	0.73	1 (9%)	13,15,17	1.24	2 (15%)
9	MAN	G	616	8	11,11,12	0.77	0	13,15,17	0.95	1 (7%)
7	NAG	G	617	4,7	14,14,15	1.72	3 (21%)	15,19,21	1.09	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	G	618	7	14,14,15	0.59	0	15,19,21	1.34	2 (13%)
7	NAG	G	619	4,7	14,14,15	0.19	0	15,19,21	0.65	1 (6%)
7	NAG	G	620	7	14,14,15	0.28	0	15,19,21	0.55	0
7	NAG	G	621	4,7	14,14,15	0.21	0	15,19,21	0.73	0
7	NAG	G	622	7	14,14,15	0.22	0	15,19,21	0.47	0
7	NAG	G	623	4,7	14,14,15	0.32	0	15,19,21	0.62	0
7	NAG	G	624	8,7	14,14,15	0.48	0	15,19,21	0.77	0
8	BMA	G	625	9,7	11,11,12	1.38	3 (27%)	13,15,17	1.30	2 (15%)
9	MAN	G	626	8	11,11,12	1.13	2 (18%)	13,15,17	1.90	5 (38%)
9	MAN	G	627	9,8	11,11,12	1.33	3 (27%)	13,15,17	2.00	3 (23%)
9	MAN	G	628	9	11,11,12	0.77	0	13,15,17	1.22	2 (15%)
7	NAG	G	629	4	14,14,15	0.42	0	15,19,21	1.37	1 (6%)
7	NAG	G	630	4,7	14,14,15	0.41	0	15,19,21	0.73	1 (6%)
7	NAG	G	631	7	14,14,15	0.28	0	15,19,21	0.55	0
7	NAG	G	632	4,7	14,14,15	0.20	0	15,19,21	0.54	0
7	NAG	G	633	7	14,14,15	0.22	0	15,19,21	0.48	0
7	NAG	G	634	4,7	14,14,15	0.96	0	15,19,21	1.82	3 (20%)
7	NAG	G	635	8,7	14,14,15	0.53	0	15,19,21	2.00	5 (33%)
8	BMA	G	636	9,7	11,11,12	0.55	0	13,15,17	1.37	2 (15%)
9	MAN	G	637	9,8	11,11,12	0.96	1 (9%)	13,15,17	2.29	4 (30%)
9	MAN	G	638	9	11,11,12	0.69	0	13,15,17	1.08	2 (15%)
9	MAN	G	639	9	11,11,12	0.75	0	13,15,17	1.38	2 (15%)
9	MAN	G	640	9,8	11,11,12	0.62	0	13,15,17	1.25	1 (7%)
9	MAN	G	641	9	11,11,12	0.98	0	13,15,17	2.56	4 (30%)
9	MAN	G	642	9	11,11,12	0.80	0	13,15,17	2.06	4 (30%)
9	MAN	G	643	9	11,11,12	0.45	0	13,15,17	2.15	2 (15%)
7	NAG	G	644	4	14,14,15	0.36	0	15,19,21	0.61	0
7	NAG	G	645	4,7	14,14,15	0.19	0	15,19,21	0.45	0
7	NAG	G	646	7	14,14,15	0.21	0	15,19,21	0.49	0
7	NAG	G	647	4,7	14,14,15	0.24	0	15,19,21	0.81	1 (6%)
7	NAG	G	648	7	14,14,15	0.29	0	15,19,21	0.53	0
7	NAG	G	649	4,7	14,14,15	0.97	1 (7%)	15,19,21	0.81	0
7	NAG	G	650	7	14,14,15	0.32	0	15,19,21	0.69	1 (6%)
7	NAG	G	651	4,7	14,14,15	0.22	0	15,19,21	0.59	0
7	NAG	G	652	7	14,14,15	0.23	0	15,19,21	0.45	0
7	NAG	G	653	4	14,14,15	0.24	0	15,19,21	0.47	0
7	NAG	H	301	5	14,14,15	0.17	0	15,19,21	0.69	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	B	701	1	-	0/6/23/26	0/1/1/1
7	NAG	B	702	1	-	0/6/23/26	0/1/1/1
7	NAG	B	703	1	-	0/6/23/26	0/1/1/1
7	NAG	G	601	4,7	-	0/6/23/26	0/1/1/1
7	NAG	G	602	8,7	-	0/6/23/26	0/1/1/1
8	BMA	G	603	9,7	-	0/2/19/22	0/1/1/1
9	MAN	G	604	8	-	0/2/19/22	0/1/1/1
9	MAN	G	605	9,8	-	0/2/19/22	0/1/1/1
9	MAN	G	606	9	-	0/2/19/22	0/1/1/1
7	NAG	G	607	4	-	0/6/23/26	0/1/1/1
7	NAG	G	608	4,7	-	0/6/23/26	0/1/1/1
7	NAG	G	609	8,7	-	0/6/23/26	0/1/1/1
8	BMA	G	610	9,7	-	0/2/19/22	0/1/1/1
9	MAN	G	611	8	-	0/2/19/22	0/1/1/1
7	NAG	G	612	4,7	-	0/6/23/26	0/1/1/1
7	NAG	G	613	8,7	-	0/6/23/26	0/1/1/1
8	BMA	G	614	9,7	-	0/2/19/22	0/1/1/1
9	MAN	G	615	8	-	0/2/19/22	0/1/1/1
9	MAN	G	616	8	-	0/2/19/22	0/1/1/1
7	NAG	G	617	4,7	-	0/6/23/26	0/1/1/1
7	NAG	G	618	7	-	0/6/23/26	0/1/1/1
7	NAG	G	619	4,7	-	0/6/23/26	0/1/1/1
7	NAG	G	620	7	-	0/6/23/26	0/1/1/1
7	NAG	G	621	4,7	-	0/6/23/26	0/1/1/1
7	NAG	G	622	7	-	0/6/23/26	0/1/1/1
7	NAG	G	623	4,7	-	0/6/23/26	0/1/1/1
7	NAG	G	624	8,7	-	0/6/23/26	0/1/1/1
8	BMA	G	625	9,7	-	0/2/19/22	0/1/1/1
9	MAN	G	626	8	-	0/2/19/22	0/1/1/1
9	MAN	G	627	9,8	-	0/2/19/22	0/1/1/1
9	MAN	G	628	9	-	0/2/19/22	1/1/1/1
7	NAG	G	629	4	-	0/6/23/26	0/1/1/1
7	NAG	G	630	4,7	-	0/6/23/26	0/1/1/1
7	NAG	G	631	7	-	0/6/23/26	0/1/1/1
7	NAG	G	632	4,7	-	0/6/23/26	0/1/1/1
7	NAG	G	633	7	-	0/6/23/26	0/1/1/1
7	NAG	G	634	4,7	-	0/6/23/26	0/1/1/1
7	NAG	G	635	8,7	-	0/6/23/26	0/1/1/1
8	BMA	G	636	9,7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MAN	G	637	9,8	-	0/2/19/22	0/1/1/1
9	MAN	G	638	9	-	0/2/19/22	0/1/1/1
9	MAN	G	639	9	-	0/2/19/22	0/1/1/1
9	MAN	G	640	9,8	-	0/2/19/22	0/1/1/1
9	MAN	G	641	9	-	0/2/19/22	0/1/1/1
9	MAN	G	642	9	-	0/2/19/22	0/1/1/1
9	MAN	G	643	9	-	0/2/19/22	0/1/1/1
7	NAG	G	644	4	-	0/6/23/26	0/1/1/1
7	NAG	G	645	4,7	-	0/6/23/26	0/1/1/1
7	NAG	G	646	7	-	0/6/23/26	0/1/1/1
7	NAG	G	647	4,7	-	0/6/23/26	0/1/1/1
7	NAG	G	648	7	-	0/6/23/26	0/1/1/1
7	NAG	G	649	4,7	-	0/6/23/26	0/1/1/1
7	NAG	G	650	7	-	0/6/23/26	0/1/1/1
7	NAG	G	651	4,7	-	0/6/23/26	0/1/1/1
7	NAG	G	652	7	-	0/6/23/26	0/1/1/1
7	NAG	G	653	4	-	0/6/23/26	0/1/1/1
7	NAG	H	301	5	-	0/6/23/26	0/1/1/1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	617	NAG	O5-C1	-5.15	1.35	1.43
7	G	649	NAG	O5-C1	-3.51	1.38	1.43
8	G	603	BMA	O5-C1	-2.23	1.40	1.43
9	G	637	MAN	C2-C3	-2.19	1.49	1.52
9	G	606	MAN	O5-C5	2.02	1.47	1.43

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	641	MAN	O2-C2-C1	-5.52	97.96	109.18
9	G	637	MAN	O5-C1-C2	-5.39	102.34	110.79
9	G	641	MAN	O5-C1-C2	-5.38	102.36	110.79
7	G	635	NAG	O5-C1-C2	-4.84	104.74	111.47
9	G	642	MAN	O2-C2-C3	-4.69	100.97	110.17

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	G	628	MAN	C1-C2-C3-C4-C5-O5

26 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	601	NAG	3	0
7	G	602	NAG	3	0
8	G	603	BMA	1	0
9	G	605	MAN	2	0
7	G	608	NAG	2	0
7	G	612	NAG	1	0
7	G	617	NAG	1	0
7	G	618	NAG	1	0
7	G	621	NAG	1	0
7	G	622	NAG	1	0
7	G	623	NAG	1	0
7	G	624	NAG	3	0
7	G	629	NAG	1	0
7	G	630	NAG	1	0
7	G	631	NAG	1	0
7	G	634	NAG	7	0
7	G	635	NAG	7	0
8	G	636	BMA	1	0
9	G	637	MAN	1	0
9	G	639	MAN	3	0
9	G	641	MAN	6	0
9	G	642	MAN	7	0
9	G	643	MAN	2	0
7	G	649	NAG	2	0
7	G	650	NAG	2	0
7	H	301	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](#)

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	B	122/153 (79%)	0.13	1 (0%) 86 82	21, 77, 141, 229	0
2	D	242/243 (99%)	1.03	48 (19%) 1 1	82, 179, 336, 392	0
3	E	213/216 (98%)	0.62	33 (15%) 2 3	89, 186, 303, 337	0
4	G	449/505 (88%)	0.10	7 (1%) 72 68	28, 80, 170, 246	0
5	H	232/235 (98%)	-0.08	1 (0%) 92 90	48, 104, 179, 228	0
6	L	208/208 (100%)	-0.10	0 100 100	35, 78, 142, 198	0
All	All	1466/1560 (93%)	0.28	90 (6%) 22 22	21, 105, 266, 392	0

The worst 5 of 90 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	216	CYS	19.6
2	D	215	SER	17.7
2	D	214	LYS	16.5
3	E	115	VAL	12.0
2	D	213	PRO	11.8

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](#)

There are no carbohydrates in this entry.

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, 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
7	NAG	G	608	14/15	0.90	0.26	1.26	108,140,173,177	0
7	NAG	B	702	14/15	0.86	0.25	0.73	156,178,188,194	0
8	BMA	G	603	11/12	0.89	0.19	0.71	78,113,127,141	0
7	NAG	G	601	14/15	0.91	0.20	-0.22	76,102,129,143	0
7	NAG	G	623	14/15	0.95	0.22	-0.42	42,73,91,100	0
9	MAN	G	640	11/12	0.95	0.17	-0.76	60,76,97,104	0
7	NAG	G	645	14/15	0.92	0.15	-0.82	106,122,146,148	0
7	NAG	G	602	14/15	0.91	0.14	-1.04	121,124,132,138	0
7	NAG	G	630	14/15	0.93	0.15	-1.08	83,102,127,127	0
7	NAG	G	624	14/15	0.95	0.18	-1.13	91,112,147,147	0
7	NAG	G	612	14/15	0.90	0.20	-1.17	59,103,114,116	0
9	MAN	G	641	11/12	0.95	0.15	-1.29	72,87,111,116	0
7	NAG	G	621	14/15	0.87	0.17	-1.53	94,149,177,180	0
7	NAG	G	634	14/15	0.94	0.15	-1.72	51,96,122,126	0
9	MAN	G	604	11/12	0.95	0.14	-	90,101,137,152	0
9	MAN	G	637	11/12	0.82	0.17	-	141,147,162,166	0
7	NAG	B	703	14/15	0.71	0.39	-	157,164,173,174	0
7	NAG	G	652	14/15	0.90	0.31	-	161,172,192,195	0
7	NAG	G	646	14/15	0.85	0.23	-	154,160,187,192	0
7	NAG	G	618	14/15	0.84	0.21	-	113,138,175,178	0
7	NAG	G	648	14/15	0.86	0.14	-	116,130,146,153	0
7	NAG	G	619	14/15	0.79	0.17	-	133,159,187,193	0
7	NAG	G	644	14/15	0.78	0.16	-	106,139,147,149	0
8	BMA	G	614	11/12	0.85	0.12	-	121,143,150,157	0
8	BMA	G	610	11/12	0.86	0.10	-	176,187,198,207	0
9	MAN	G	626	11/12	0.88	0.13	-	103,117,139,141	0
7	NAG	G	650	14/15	0.86	0.39	-	150,172,182,188	0
9	MAN	G	642	11/12	0.96	0.12	-	98,116,138,147	0
8	BMA	G	636	11/12	0.95	0.16	-	102,130,146,147	0
9	MAN	G	616	11/12	0.83	0.14	-	125,144,153,154	0
7	NAG	G	629	14/15	0.82	0.32	-	141,150,156,167	0
7	NAG	G	622	14/15	0.82	0.57	-	175,193,201,202	0
9	MAN	G	606	11/12	0.93	0.15	-	137,141,157,167	0
9	MAN	G	628	11/12	0.88	0.15	-	151,168,188,200	0
9	MAN	G	615	11/12	0.90	0.20	-	108,121,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	NAG	H	301	14/15	0.63	0.33	-	189,207,211,211	0
9	MAN	G	611	11/12	0.91	0.32	-	140,169,187,189	0
9	MAN	G	643	11/12	0.89	0.15	-	154,182,188,190	0
9	MAN	G	605	11/12	0.86	0.17	-	138,154,176,182	0
7	NAG	G	631	14/15	0.89	0.20	-	108,129,138,138	0
7	NAG	G	617	14/15	0.95	0.13	-	93,109,128,135	0
7	NAG	G	607	14/15	0.85	0.19	-	94,114,126,137	0
7	NAG	G	633	14/15	0.82	0.23	-	137,151,165,171	0
8	BMA	G	625	11/12	0.93	0.11	-	125,141,151,160	0
7	NAG	G	635	14/15	0.94	0.16	-	107,122,133,141	0
7	NAG	G	649	14/15	0.92	0.28	-	123,161,167,173	0
9	MAN	G	639	11/12	0.94	0.14	-	149,153,163,174	0
9	MAN	G	627	11/12	0.90	0.13	-	115,135,152,174	0
7	NAG	G	651	14/15	0.88	0.17	-	74,132,158,161	0
7	NAG	G	613	14/15	0.90	0.17	-	118,131,139,146	0
7	NAG	G	609	14/15	0.89	0.11	-	116,144,163,180	0
7	NAG	G	620	14/15	0.69	0.38	-	178,208,220,224	0
7	NAG	G	653	14/15	0.83	0.26	-	161,201,208,213	0
7	NAG	G	632	14/15	0.95	0.25	-	68,106,128,130	0
7	NAG	G	647	14/15	0.95	0.16	-	94,123,148,151	0
7	NAG	B	701	14/15	0.76	0.26	-	176,194,207,212	0
9	MAN	G	638	11/12	0.82	0.17	-	154,157,159,160	0

6.5 Other polymers [i](#)

There are no such residues in this entry.