



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2018 – 04:44 PM EDT

PDB ID : 6B0N
Title : Crystal structure of the cleavage-independent prefusion HIV Env glycoprotein trimer of the clade A BG505 isolate (NFL construct) in complex with Fabs PGT122 and PGV19 at 3.39 Å
Authors : Sarkar, A.; Irimia, A.; Wilson, I.A.
Deposited on : 2017-09-14
Resolution : 3.40 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	:	rb-20031021
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)	:	rb-20031021

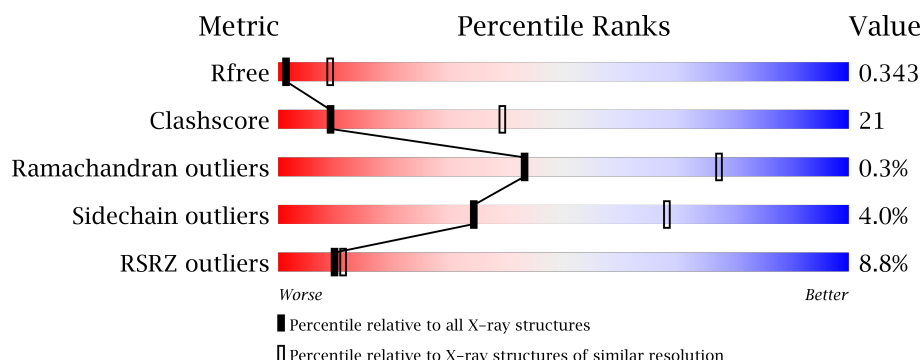
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1928 (3.50-3.30)
Clashscore	122126	2051 (3.50-3.30)
Ramachandran outliers	120053	2006 (3.50-3.30)
Sidechain outliers	120020	2006 (3.50-3.30)
RSRZ outliers	108989	1827 (3.50-3.30)

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	D	223	<div> <div>10%</div> <div> <div>52%</div> <div>22%</div> <div>•</div> <div>23%</div> </div> </div>
2	E	209	<div> <div>19%</div> <div> <div>73%</div> <div>13%</div> <div>13%</div> </div> </div>
3	G	638	<div> <div>5%</div> <div> <div>64%</div> <div>28%</div> <div>• •</div> </div> </div>
4	H	235	<div> <div>6%</div> <div> <div>74%</div> <div>22%</div> <div>• •</div> </div> </div>
5	L	213	<div> <div>8%</div> <div> <div>72%</div> <div>25%</div> <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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MAN	G	1265	-	-	X	-
6	MAN	G	1266	-	-	X	X
6	MAN	G	1267	-	-	-	X
6	MAN	G	1269	-	-	-	X
6	MAN	G	1337	-	-	X	-
7	NAG	G	1133	-	-	X	-
7	NAG	G	1235	-	-	-	X
7	NAG	G	1355	-	-	-	X
7	NAG	G	1363	-	-	X	-
7	NAG	G	1386	-	-	X	-
7	NAG	G	1387	-	-	X	-
7	NAG	G	1840	-	-	-	X
8	BMA	G	1333	-	-	X	-
8	BMA	G	1388	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11789 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 PGV19 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	171	Total	C	N	O	S	0	0	0
			1341	851	237	244	9			

- Molecule 2 is a protein called PGV19 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	182	Total	C	N	O	S	0	0	0
			1375	866	233	272	4			

- Molecule 3 is a protein called Envelope glycoprotein gp140.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	610	Total	C	N	O	S	0	0	0
			4754	2992	832	898	32			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	ASN	THR	engineered mutation	UNP Q2N0S6
G	507	GLY	-	linker	UNP Q2N0S6
G	508	GLY	-	linker	UNP Q2N0S6
G	509	GLY	-	linker	UNP Q2N0S6
G	509A	GLY	-	linker	UNP Q2N0S6
G	509B	GLY	-	linker	UNP Q2N0S6
G	509C	SER	-	linker	UNP Q2N0S6
G	509D	GLY	-	linker	UNP Q2N0S6
G	509E	GLY	-	linker	UNP Q2N0S6
G	509F	GLY	-	linker	UNP Q2N0S6
G	509G	GLY	-	linker	UNP Q2N0S6
G	511	SER	-	linker	UNP Q2N0S6
G	559	PRO	ILE	engineered mutation	UNP Q2N0S9

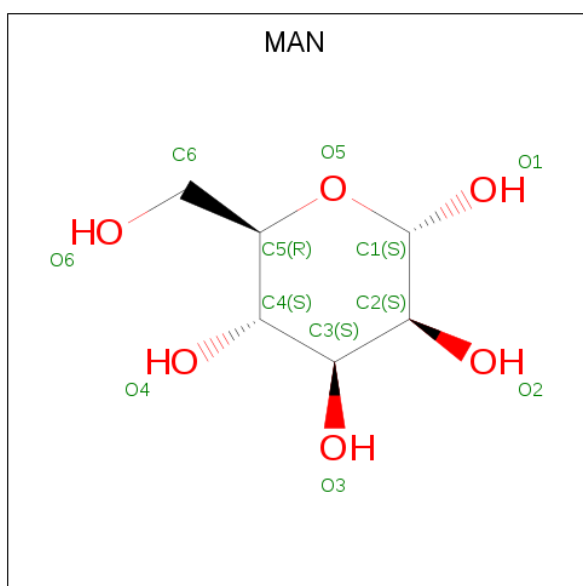
- Molecule 4 is a protein called PGT122 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	232	Total	C	N	O	S	0	0	0
			1767	1122	300	340	5			

- Molecule 5 is a protein called PGT122 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	210	Total	C	N	O	S	0	0	0
			1586	997	266	319	4			

- Molecule 6 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



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

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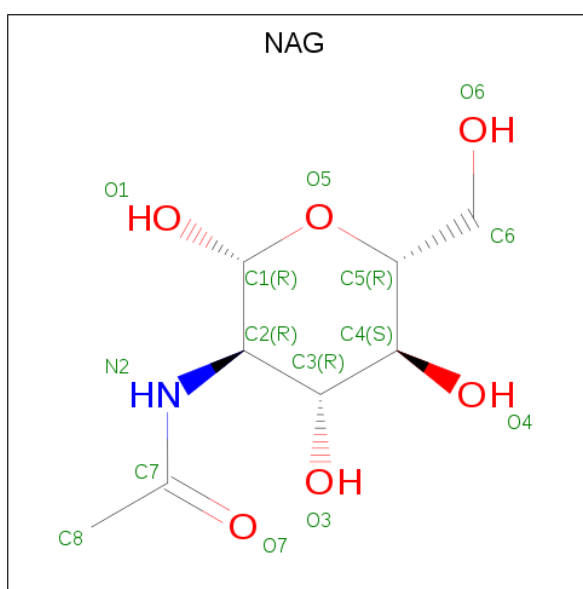
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	C	O	0	0
			11	6	5		
6	G	1	Total	C	O	0	0
			11	6	5		
6	G	1	Total	C	O	0	0
			11	6	5		
6	G	1	Total	C	O	0	0
			11	6	5		
6	G	1	Total	C	O	0	0
			11	6	5		
6	G	1	Total	C	O	0	0
			11	6	5		
6	G	1	Total	C	O	0	0
			11	6	5		
6	G	1	Total	C	O	0	0
			11	6	5		
6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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	C	O	0	0
			11	6	5		
6	G	1	Total	C	O	0	0
			11	6	5		
6	G	1	Total	C	O	0	0
			11	6	5		
6	G	1	Total	C	O	0	0
			11	6	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	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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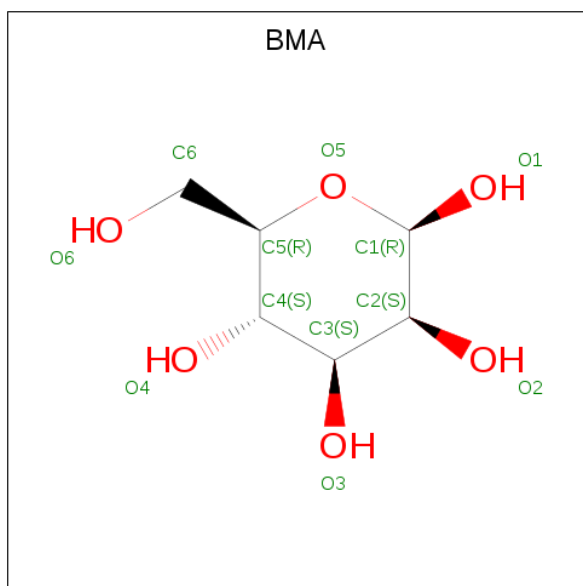
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	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	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		

- 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		

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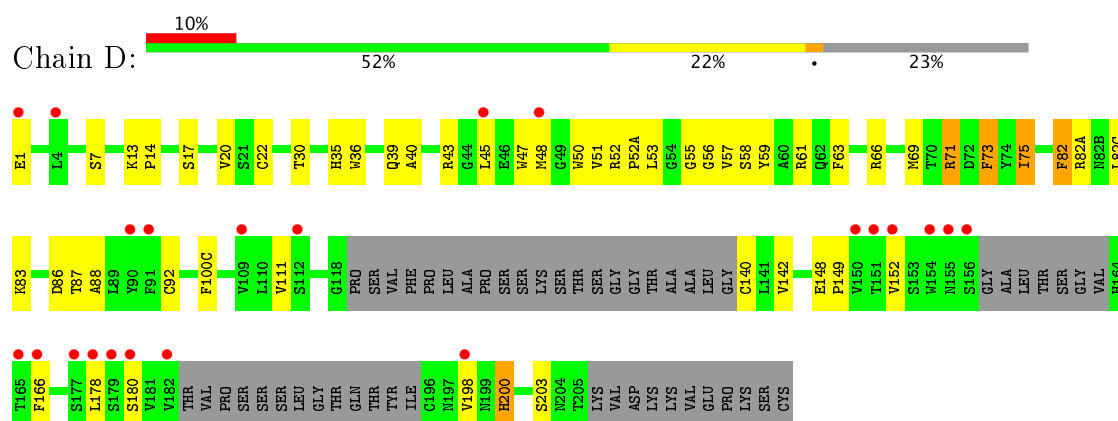
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	G	1	Total	C	O	0	0
			11	6	5		
8	G	1	Total	C	O	0	0
			11	6	5		
8	G	1	Total	C	O	0	0
			11	6	5		
8	G	1	Total	C	O	0	0
			11	6	5		
8	G	1	Total	C	O	0	0
			11	6	5		
8	G	1	Total	C	O	0	0
			11	6	5		

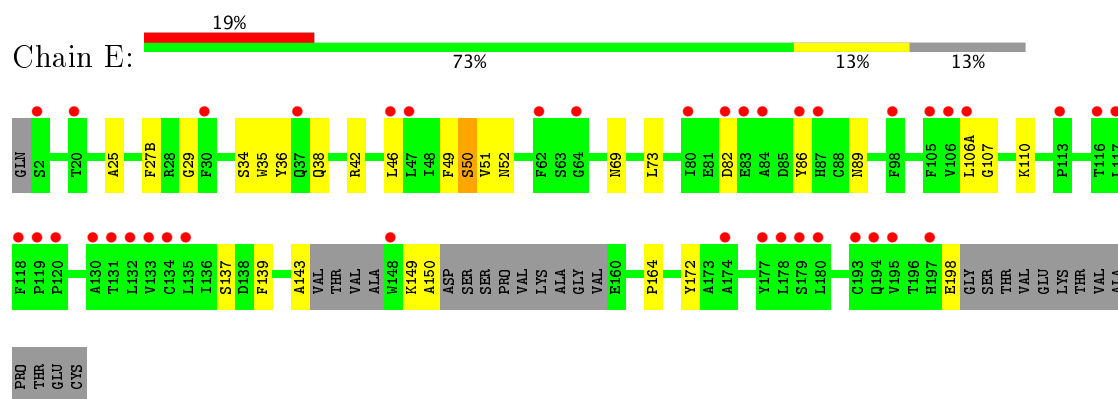
3 Residue-property plots [i](#)

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.

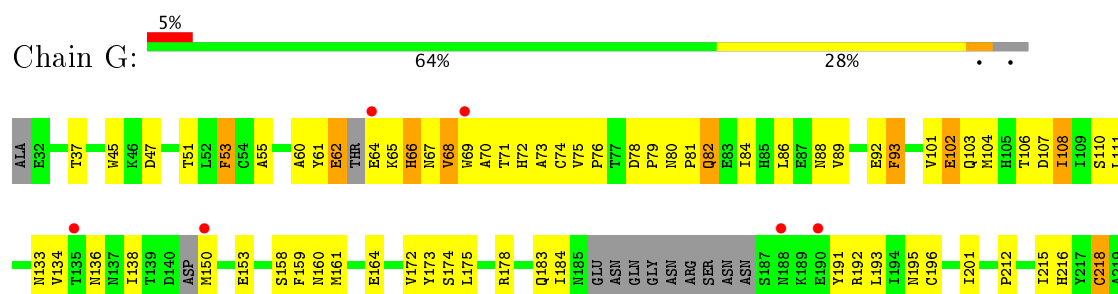
• Molecule 1: PGV19 Fab heavy chain

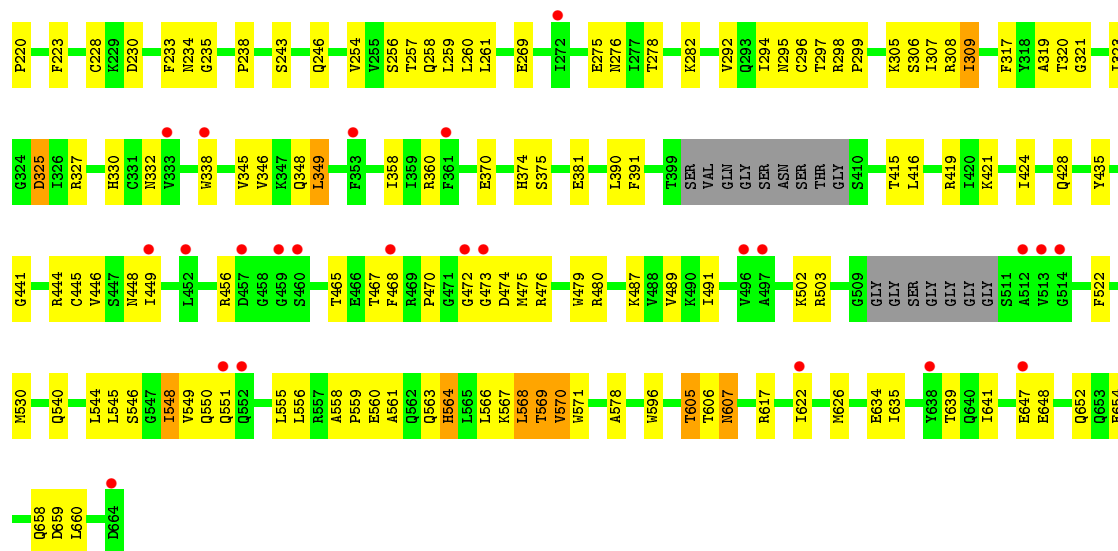


• Molecule 2: PGV19 light chain

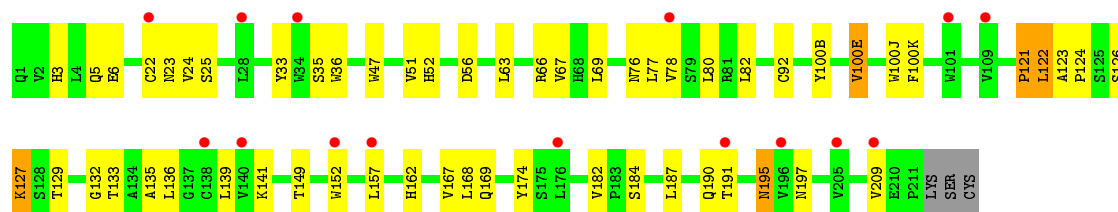
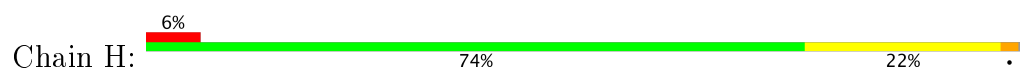


• Molecule 3: Envelope glycoprotein gp140

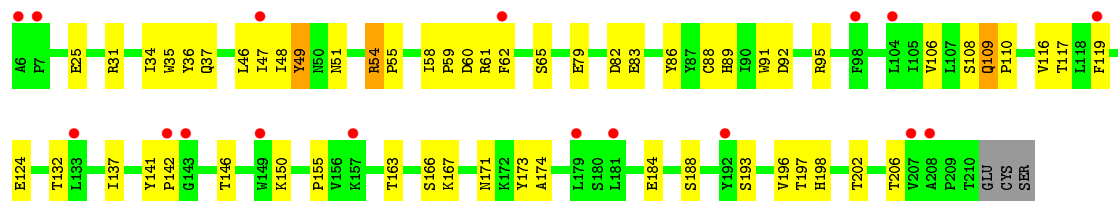




• Molecule 4: PGT122 Fab heavy chain



• Molecule 5: PGT122 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	161.25Å 161.25Å 245.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.85 – 3.40 48.85 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.85-3.40) 98.6 (48.85-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.21	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.12_2829: 000)	Depositor
R, R_{free}	0.335 , 0.346 0.335 , 0.343	Depositor DCC
R_{free} test set	2458 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	91.9	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , -10.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.066 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	11789	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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	D	0.33	0/1375	0.50	0/1861
2	E	0.28	0/1410	0.50	0/1914
3	G	0.40	0/4847	0.59	0/6582
4	H	0.32	0/1815	0.49	0/2479
5	L	0.33	0/1629	0.55	0/2232
All	All	0.36	0/11076	0.55	0/15068

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	D	1341	0	1285	69	0
2	E	1375	0	1320	19	0
3	G	4754	0	4644	232	1
4	H	1767	0	1738	64	0
5	L	1586	0	1526	72	0
6	G	352	0	304	26	0
7	G	504	0	443	46	0
8	G	110	0	83	18	0
All	All	11789	0	11343	493	1

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 21.

The worst 5 of 493 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:G:133:ASN:HD21	7:G:1133:NAG:C1	1.06	1.63
3:G:64:GLU:HB2	3:G:66:HIS:CE1	1.37	1.55
5:L:35:TRP:CD1	5:L:48:ILE:HD11	1.45	1.52
3:G:64:GLU:CB	3:G:66:HIS:CE1	1.89	1.51
3:G:325:ASP:OD2	4:H:100(B):TYR:CD1	1.70	1.44

All (1) 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)
3:G:103:GLN:NE2	3:G:560:GLU:OE2[3_685]	1.96	0.24

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	D	163/223 (73%)	157 (96%)	6 (4%)	0	100	100
2	E	176/209 (84%)	171 (97%)	5 (3%)	0	100	100
3	G	598/638 (94%)	572 (96%)	25 (4%)	1 (0%)	49	82
4	H	230/235 (98%)	222 (96%)	6 (3%)	2 (1%)	19	58
5	L	208/213 (98%)	201 (97%)	6 (3%)	1 (0%)	31	69
All	All	1375/1518 (91%)	1323 (96%)	48 (4%)	4 (0%)	43	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	100(E)	VAL
5	L	109	GLN
3	G	570	VAL
4	H	121	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	D	142/185 (77%)	136 (96%)	6 (4%)	32	67
2	E	153/176 (87%)	150 (98%)	3 (2%)	58	82
3	G	527/552 (96%)	500 (95%)	27 (5%)	26	61
4	H	201/205 (98%)	192 (96%)	9 (4%)	30	66
5	L	177/181 (98%)	174 (98%)	3 (2%)	63	84
All	All	1200/1299 (92%)	1152 (96%)	48 (4%)	34	68

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	218	CYS
3	G	548	ILE
4	H	195	ASN
3	G	307	ILE
3	G	325	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
3	G	216	HIS
5	L	109	GLN
3	G	246	GLN
1	D	64	GLN
3	G	348	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 ⓘ

78 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	MAN	G	1060	6	11,11,12	0.46	0	15,15,17	0.81	0
7	NAG	G	1088	3	14,14,15	0.40	0	17,19,21	1.17	1 (5%)
7	NAG	G	1133	-	14,14,15	0.41	0	17,19,21	1.17	2 (11%)
7	NAG	G	1137	3	14,14,15	0.59	0	17,19,21	0.82	0
7	NAG	G	1156	3,7	14,14,15	0.52	0	17,19,21	0.88	0
7	NAG	G	1157	8,7	14,14,15	0.50	0	17,19,21	0.82	0
8	BMA	G	1158	7,6	11,11,12	0.35	0	15,15,17	0.75	0
6	MAN	G	1159	8,6	11,11,12	0.48	0	15,15,17	0.78	0
7	NAG	G	1160	3,7	14,14,15	0.60	0	17,19,21	0.76	0
7	NAG	G	1161	8,7	14,14,15	0.86	0	17,19,21	1.81	2 (11%)
8	BMA	G	1162	7	11,11,12	0.44	0	15,15,17	0.64	0
6	MAN	G	1169	8,6	11,11,12	0.41	0	15,15,17	0.91	1 (6%)
6	MAN	G	1170	6	11,11,12	0.40	0	15,15,17	1.13	1 (6%)
7	NAG	G	1197	3,7	14,14,15	0.25	0	17,19,21	0.53	0
7	NAG	G	1198	8,7	14,14,15	0.32	0	17,19,21	0.68	0
8	BMA	G	1199	7	11,11,12	1.06	1 (9%)	15,15,17	1.22	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	G	1201	-	11,11,12	0.57	0	15,15,17	3.37	4 (26%)
7	NAG	G	1234	-	14,14,15	0.41	0	17,19,21	1.19	1 (5%)
7	NAG	G	1235	-	14,14,15	0.55	0	17,19,21	0.87	0
7	NAG	G	1262	3,7	14,14,15	0.47	0	17,19,21	0.86	0
7	NAG	G	1263	8,7	14,14,15	0.53	0	17,19,21	0.90	0
8	BMA	G	1264	7,6	11,11,12	0.47	0	15,15,17	0.79	0
6	MAN	G	1265	8,6	11,11,12	0.39	0	15,15,17	0.81	0
6	MAN	G	1266	-	11,11,12	0.35	0	15,15,17	0.78	0
6	MAN	G	1267	6	11,11,12	0.40	0	15,15,17	1.13	1 (6%)
6	MAN	G	1268	8,6	11,11,12	0.43	0	15,15,17	1.25	2 (13%)
6	MAN	G	1269	6	11,11,12	0.46	0	15,15,17	1.97	4 (26%)
6	MAN	G	1270	6	11,11,12	0.45	0	15,15,17	1.22	1 (6%)
7	NAG	G	1276	3,7	14,14,15	0.81	0	17,19,21	1.75	3 (17%)
7	NAG	G	1277	8,7	14,14,15	0.66	0	17,19,21	1.04	0
8	BMA	G	1278	7,6	11,11,12	0.79	0	15,15,17	0.93	2 (13%)
6	MAN	G	1279	8	11,11,12	0.44	0	15,15,17	0.66	0
6	MAN	G	1280	8	11,11,12	0.62	0	15,15,17	0.80	0
7	NAG	G	1295	3,7	14,14,15	0.47	0	17,19,21	0.78	0
7	NAG	G	1296	7	14,14,15	0.56	0	17,19,21	0.88	0
7	NAG	G	1301	3,7	14,14,15	0.55	0	17,19,21	0.95	1 (5%)
7	NAG	G	1302	8,7	14,14,15	0.57	0	17,19,21	0.85	0
8	BMA	G	1303	7,6	11,11,12	0.50	0	15,15,17	0.71	0
6	MAN	G	1309	8	11,11,12	0.53	0	15,15,17	0.78	0
7	NAG	G	1331	3,7	14,14,15	0.32	0	17,19,21	0.49	0
7	NAG	G	1332	8,7	14,14,15	0.38	0	17,19,21	0.67	0
8	BMA	G	1333	7,6	11,11,12	0.62	0	15,15,17	0.87	0
6	MAN	G	1334	8,6	11,11,12	0.79	0	15,15,17	1.76	3 (20%)
6	MAN	G	1335	6	11,11,12	0.44	0	15,15,17	0.81	0
6	MAN	G	1336	6	11,11,12	0.37	0	15,15,17	1.12	1 (6%)
6	MAN	G	1337	6	11,11,12	0.39	0	15,15,17	0.73	0
6	MAN	G	1338	6	11,11,12	0.40	0	15,15,17	0.81	0
6	MAN	G	1339	6	11,11,12	0.41	0	15,15,17	0.76	0
6	MAN	G	1340	6	11,11,12	0.54	0	15,15,17	1.06	2 (13%)
6	MAN	G	1341	6	11,11,12	0.43	0	15,15,17	0.73	0
7	NAG	G	1355	3	14,14,15	0.42	0	17,19,21	0.84	0
7	NAG	G	1363	3,7	14,14,15	0.62	0	17,19,21	0.91	0
7	NAG	G	1364	8,7	14,14,15	0.60	0	17,19,21	2.68	5 (29%)
8	BMA	G	1365	7,6	11,11,12	0.79	1 (9%)	15,15,17	1.73	4 (26%)
6	MAN	G	1366	8	11,11,12	0.62	0	15,15,17	1.03	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	G	1367	8	11,11,12	0.48	0	15,15,17	1.29	3 (20%)
7	NAG	G	1386	3,7	14,14,15	0.40	0	17,19,21	1.17	2 (11%)
7	NAG	G	1387	7	14,14,15	0.77	0	17,19,21	0.87	0
8	BMA	G	1388	6	11,11,12	0.59	0	15,15,17	1.13	1 (6%)
6	MAN	G	1389	8	11,11,12	0.56	0	15,15,17	2.75	4 (26%)
6	MAN	G	1390	8,6	11,11,12	0.43	0	15,15,17	0.79	0
6	MAN	G	1391	6	11,11,12	0.45	0	15,15,17	0.80	0
7	NAG	G	1392	3,7	14,14,15	0.62	0	17,19,21	0.92	0
7	NAG	G	1393	7	14,14,15	0.70	0	17,19,21	0.86	0
7	NAG	G	1448	3,7	14,14,15	0.53	0	17,19,21	0.88	0
7	NAG	G	1449	8,7	14,14,15	0.59	0	17,19,21	0.92	1 (5%)
8	BMA	G	1450	7,6	11,11,12	0.34	0	15,15,17	1.52	4 (26%)
6	MAN	G	1451	8,6	11,11,12	0.43	0	15,15,17	0.69	0
6	MAN	G	1452	8,6	11,11,12	0.42	0	15,15,17	1.10	0
6	MAN	G	1453	6	11,11,12	0.29	0	15,15,17	0.83	0
6	MAN	G	1454	6	11,11,12	0.42	0	15,15,17	1.02	0
6	MAN	G	1455	6	11,11,12	0.43	0	15,15,17	0.68	0
7	NAG	G	1611	3	14,14,15	0.59	0	17,19,21	1.04	0
7	NAG	G	1618	3	14,14,15	0.61	0	17,19,21	0.79	0
7	NAG	G	1625	3	14,14,15	0.40	0	17,19,21	1.17	1 (5%)
7	NAG	G	1637	3	14,14,15	0.53	0	17,19,21	0.92	0
7	NAG	G	1839	3	14,14,15	0.58	0	17,19,21	0.82	0
7	NAG	G	1840	3	14,14,15	0.96	0	17,19,21	1.67	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	G	1060	6	-	0/2/19/22	0/1/1/1
7	NAG	G	1088	3	-	0/6/23/26	0/1/1/1
7	NAG	G	1133	-	-	0/6/23/26	0/1/1/1
7	NAG	G	1137	3	-	0/6/23/26	0/1/1/1
7	NAG	G	1156	3,7	-	0/6/23/26	0/1/1/1
7	NAG	G	1157	8,7	-	0/6/23/26	0/1/1/1
8	BMA	G	1158	7,6	-	0/2/19/22	0/1/1/1
6	MAN	G	1159	8,6	-	0/2/19/22	0/1/1/1
7	NAG	G	1160	3,7	-	0/6/23/26	0/1/1/1
7	NAG	G	1161	8,7	-	0/6/23/26	0/1/1/1
8	BMA	G	1162	7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	G	1169	8,6	-	0/2/19/22	0/1/1/1
6	MAN	G	1170	6	-	0/2/19/22	0/1/1/1
7	NAG	G	1197	3,7	-	0/6/23/26	0/1/1/1
7	NAG	G	1198	8,7	-	0/6/23/26	0/1/1/1
8	BMA	G	1199	7	-	0/2/19/22	0/1/1/1
6	MAN	G	1201	-	-	0/2/19/22	0/1/1/1
7	NAG	G	1234	-	-	0/6/23/26	0/1/1/1
7	NAG	G	1235	-	-	0/6/23/26	0/1/1/1
7	NAG	G	1262	3,7	-	0/6/23/26	0/1/1/1
7	NAG	G	1263	8,7	-	0/6/23/26	0/1/1/1
8	BMA	G	1264	7,6	-	0/2/19/22	0/1/1/1
6	MAN	G	1265	8,6	-	0/2/19/22	0/1/1/1
6	MAN	G	1266	-	-	0/2/19/22	0/1/1/1
6	MAN	G	1267	6	-	0/2/19/22	0/1/1/1
6	MAN	G	1268	8,6	-	0/2/19/22	0/1/1/1
6	MAN	G	1269	6	-	0/2/19/22	0/1/1/1
6	MAN	G	1270	6	-	0/2/19/22	0/1/1/1
7	NAG	G	1276	3,7	-	0/6/23/26	0/1/1/1
7	NAG	G	1277	8,7	-	0/6/23/26	0/1/1/1
8	BMA	G	1278	7,6	-	0/2/19/22	0/1/1/1
6	MAN	G	1279	8	-	0/2/19/22	0/1/1/1
6	MAN	G	1280	8	-	0/2/19/22	0/1/1/1
7	NAG	G	1295	3,7	-	0/6/23/26	0/1/1/1
7	NAG	G	1296	7	-	0/6/23/26	0/1/1/1
7	NAG	G	1301	3,7	-	0/6/23/26	0/1/1/1
7	NAG	G	1302	8,7	-	0/6/23/26	0/1/1/1
8	BMA	G	1303	7,6	-	0/2/19/22	0/1/1/1
6	MAN	G	1309	8	-	0/2/19/22	0/1/1/1
7	NAG	G	1331	3,7	-	0/6/23/26	0/1/1/1
7	NAG	G	1332	8,7	-	0/6/23/26	0/1/1/1
8	BMA	G	1333	7,6	-	0/2/19/22	0/1/1/1
6	MAN	G	1334	8,6	-	0/2/19/22	0/1/1/1
6	MAN	G	1335	6	-	0/2/19/22	0/1/1/1
6	MAN	G	1336	6	-	0/2/19/22	0/1/1/1
6	MAN	G	1337	6	-	0/2/19/22	0/1/1/1
6	MAN	G	1338	6	-	0/2/19/22	0/1/1/1
6	MAN	G	1339	6	-	0/2/19/22	0/1/1/1
6	MAN	G	1340	6	-	0/2/19/22	0/1/1/1
6	MAN	G	1341	6	-	0/2/19/22	0/1/1/1
7	NAG	G	1355	3	-	0/6/23/26	0/1/1/1
7	NAG	G	1363	3,7	-	0/6/23/26	0/1/1/1
7	NAG	G	1364	8,7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BMA	G	1365	7,6	-	0/2/19/22	0/1/1/1
6	MAN	G	1366	8	-	0/2/19/22	0/1/1/1
6	MAN	G	1367	8	-	0/2/19/22	0/1/1/1
7	NAG	G	1386	3,7	-	0/6/23/26	0/1/1/1
7	NAG	G	1387	7	-	0/6/23/26	0/1/1/1
8	BMA	G	1388	6	-	0/2/19/22	0/1/1/1
6	MAN	G	1389	8	-	0/2/19/22	0/1/1/1
6	MAN	G	1390	8,6	-	0/2/19/22	0/1/1/1
6	MAN	G	1391	6	-	0/2/19/22	0/1/1/1
7	NAG	G	1392	3,7	-	0/6/23/26	0/1/1/1
7	NAG	G	1393	7	-	0/6/23/26	0/1/1/1
7	NAG	G	1448	3,7	-	0/6/23/26	0/1/1/1
7	NAG	G	1449	8,7	-	0/6/23/26	0/1/1/1
8	BMA	G	1450	7,6	-	0/2/19/22	0/1/1/1
6	MAN	G	1451	8,6	-	0/2/19/22	0/1/1/1
6	MAN	G	1452	8,6	-	0/2/19/22	0/1/1/1
6	MAN	G	1453	6	-	0/2/19/22	0/1/1/1
6	MAN	G	1454	6	-	0/2/19/22	0/1/1/1
6	MAN	G	1455	6	-	0/2/19/22	0/1/1/1
7	NAG	G	1611	3	-	0/6/23/26	0/1/1/1
7	NAG	G	1618	3	-	0/6/23/26	0/1/1/1
7	NAG	G	1625	3	-	0/6/23/26	0/1/1/1
7	NAG	G	1637	3	-	0/6/23/26	0/1/1/1
7	NAG	G	1839	3	-	0/6/23/26	0/1/1/1
7	NAG	G	1840	3	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	1365	BMA	O5-C1	-2.14	1.40	1.43
8	G	1199	BMA	C2-C3	2.18	1.55	1.52

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	1364	NAG	O3-C3-C2	-6.45	95.57	109.39
6	G	1389	MAN	O3-C3-C4	-5.89	96.59	110.34
6	G	1201	MAN	O3-C3-C4	-5.87	96.63	110.34
6	G	1201	MAN	O4-C4-C5	-5.71	95.01	109.31
6	G	1389	MAN	O4-C4-C5	-5.70	95.03	109.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

25 monomers are involved in 72 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	1088	NAG	1	0
7	G	1133	NAG	8	0
7	G	1137	NAG	1	0
7	G	1156	NAG	1	0
7	G	1160	NAG	1	0
8	G	1199	BMA	2	0
6	G	1201	MAN	2	0
7	G	1234	NAG	2	0
7	G	1235	NAG	2	0
7	G	1262	NAG	1	0
7	G	1263	NAG	1	0
8	G	1264	BMA	1	0
6	G	1265	MAN	14	0
6	G	1266	MAN	14	0
6	G	1268	MAN	1	0
7	G	1277	NAG	1	0
7	G	1331	NAG	2	0
8	G	1333	BMA	9	0
6	G	1337	MAN	9	0
7	G	1363	NAG	18	0
7	G	1364	NAG	1	0
7	G	1386	NAG	20	0
7	G	1387	NAG	9	0
8	G	1388	BMA	6	0
7	G	1448	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	D	171/223 (76%)	0.55	22 (12%) 3 4	81, 125, 206, 214	0
2	E	182/209 (87%)	1.01	40 (21%) 0 1	130, 168, 244, 255	0
3	G	610/638 (95%)	0.39	30 (4%) 29 29	58, 91, 145, 196	2 (0%)
4	H	232/235 (98%)	0.25	15 (6%) 19 20	96, 123, 149, 161	0
5	L	210/213 (98%)	0.32	17 (8%) 12 13	90, 119, 177, 199	0
All	All	1405/1518 (92%)	0.45	124 (8%) 10 11	58, 115, 211, 255	2 (0%)

The worst 5 of 124 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	179	SER	11.7
2	E	133	VAL	8.0
3	G	150	MET	7.1
5	L	6	ALA	6.6
2	E	120	PRO	6.3

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 [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. 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	B-factors(Å ²)	Q<0.9
8	BMA	G	1199	11/12	0.34	0.26	171,177,190,195	0
6	MAN	G	1269	11/12	0.54	0.47	126,128,129,129	11
6	MAN	G	1265	11/12	0.55	0.29	151,153,155,156	11
6	MAN	G	1266	11/12	0.61	0.46	126,128,129,129	11
8	BMA	G	1278	11/12	0.64	0.20	157,158,162,162	0
7	NAG	G	1088	14/15	0.66	0.29	53,53,53,53	0
8	BMA	G	1303	11/12	0.67	0.23	148,150,153,154	0
6	MAN	G	1279	11/12	0.67	0.32	153,155,157,157	11
7	NAG	G	1840	14/15	0.68	0.63	130,132,133,133	0
8	BMA	G	1264	11/12	0.70	0.36	143,144,147,149	11
6	MAN	G	1455	11/12	0.70	0.27	161,162,163,163	11
7	NAG	G	1355	14/15	0.70	0.44	63,63,63,63	14
6	MAN	G	1451	11/12	0.70	0.36	157,158,159,160	11
6	MAN	G	1309	11/12	0.72	0.25	145,147,150,150	0
7	NAG	G	1235	14/15	0.72	0.44	152,153,156,158	14
7	NAG	G	1839	14/15	0.72	0.30	159,165,169,170	0
6	MAN	G	1452	11/12	0.72	0.13	159,160,162,163	0
8	BMA	G	1333	11/12	0.73	0.16	84,102,116,128	0
6	MAN	G	1267	11/12	0.74	0.42	53,53,53,53	0
6	MAN	G	1201	11/12	0.75	0.37	39,39,39,39	0
7	NAG	G	1137	14/15	0.75	0.31	132,135,138,139	0
7	NAG	G	1363	14/15	0.76	0.26	142,144,145,146	0
7	NAG	G	1133	14/15	0.77	0.25	53,53,53,53	0
7	NAG	G	1277	14/15	0.77	0.36	156,159,161,163	14
6	MAN	G	1391	11/12	0.77	0.21	144,152,155,158	0
7	NAG	G	1387	14/15	0.77	0.24	141,142,143,143	0
7	NAG	G	1625	14/15	0.78	0.36	53,53,53,53	0
7	NAG	G	1449	14/15	0.79	0.17	154,155,157,157	0
6	MAN	G	1280	11/12	0.79	0.34	161,163,165,166	0
8	BMA	G	1162	11/12	0.80	0.28	138,140,141,141	0
8	BMA	G	1450	11/12	0.80	0.11	157,159,160,160	0
6	MAN	G	1341	11/12	0.81	0.27	155,160,166,168	11
7	NAG	G	1198	14/15	0.81	0.31	136,151,158,165	0
8	BMA	G	1388	11/12	0.82	0.19	39,39,39,39	0
7	NAG	G	1161	14/15	0.82	0.25	136,136,138,139	0
7	NAG	G	1392	14/15	0.82	0.21	142,150,157,158	0
6	MAN	G	1389	11/12	0.82	0.25	39,39,39,39	0
7	NAG	G	1393	14/15	0.83	0.17	157,159,161,162	0
7	NAG	G	1197	14/15	0.83	0.28	123,140,152,157	0
6	MAN	G	1060	11/12	0.83	0.24	133,134,135,137	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	NAG	G	1276	14/15	0.84	0.23	154,157,161,162	0
6	MAN	G	1169	11/12	0.84	0.13	136,136,139,139	0
6	MAN	G	1340	11/12	0.84	0.21	39,39,39,39	11
6	MAN	G	1270	11/12	0.84	0.29	39,39,39,39	0
6	MAN	G	1454	11/12	0.84	0.29	39,39,39,39	0
6	MAN	G	1339	11/12	0.84	0.30	142,143,147,150	0
6	MAN	G	1390	11/12	0.85	0.22	152,155,159,159	11
7	NAG	G	1160	14/15	0.85	0.19	133,134,135,135	0
7	NAG	G	1386	14/15	0.85	0.18	53,53,53,53	0
7	NAG	G	1611	14/15	0.86	0.27	157,160,162,162	0
7	NAG	G	1234	14/15	0.86	0.23	53,53,53,53	0
7	NAG	G	1332	14/15	0.86	0.22	61,89,109,117	0
7	NAG	G	1618	14/15	0.87	0.18	170,176,181,184	0
6	MAN	G	1336	11/12	0.87	0.24	150,152,158,158	11
8	BMA	G	1365	11/12	0.87	0.10	53,53,53,53	0
7	NAG	G	1364	14/15	0.88	0.15	39,39,39,39	0
7	NAG	G	1448	14/15	0.88	0.19	149,150,153,153	0
6	MAN	G	1334	11/12	0.88	0.13	147,149,152,154	0
6	MAN	G	1170	11/12	0.89	0.29	53,53,53,53	0
6	MAN	G	1337	11/12	0.89	0.26	134,136,138,138	0
6	MAN	G	1453	11/12	0.89	0.13	157,158,159,159	0
7	NAG	G	1331	14/15	0.89	0.16	87,106,110,121	0
7	NAG	G	1302	14/15	0.89	0.14	140,143,146,146	0
6	MAN	G	1366	11/12	0.90	0.23	39,39,39,39	0
6	MAN	G	1268	11/12	0.90	0.32	136,140,142,142	11
7	NAG	G	1296	14/15	0.91	0.12	146,148,151,152	0
7	NAG	G	1157	14/15	0.91	0.19	130,131,132,132	0
7	NAG	G	1156	14/15	0.91	0.28	128,129,130,130	0
7	NAG	G	1637	14/15	0.91	0.21	155,156,158,159	0
7	NAG	G	1295	14/15	0.92	0.17	138,142,145,146	0
6	MAN	G	1338	11/12	0.92	0.20	139,140,143,145	0
6	MAN	G	1367	11/12	0.93	0.18	141,146,148,149	0
6	MAN	G	1159	11/12	0.93	0.16	133,134,135,135	0
8	BMA	G	1158	11/12	0.93	0.07	132,134,135,135	0
6	MAN	G	1335	11/12	0.93	0.14	155,159,162,164	0
7	NAG	G	1301	14/15	0.93	0.19	136,137,140,140	0
7	NAG	G	1263	14/15	0.93	0.19	138,144,151,153	0
7	NAG	G	1262	14/15	0.95	0.27	136,142,148,149	0

6.5 Other polymers ⓘ

There are no such residues in this entry.