



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 25, 2016 – 05:54 AM EDT

PDB ID : 5T3S  
Title : HIV gp140 trimer MD39-10MUTA in complex with Fabs PGT124 and 35022  
Authors : Stanfield, R.L.; Wilson, I.A.  
Deposited on : 2016-08-26  
Resolution : 4.50 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

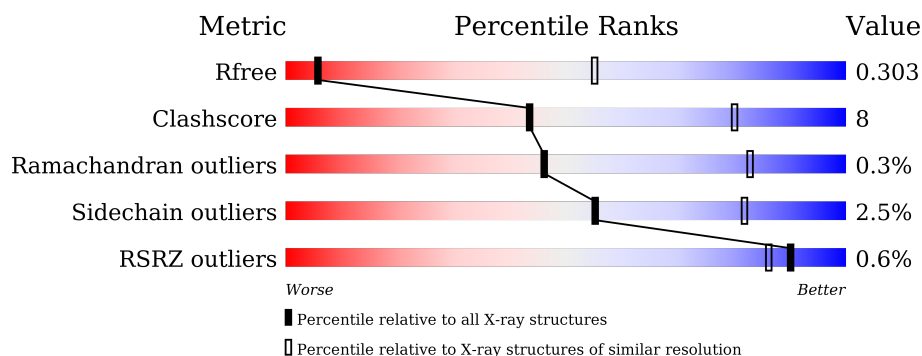
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1071 (5.40-3.60)
Clashscore	102246	1003 (5.30-3.62)
Ramachandran outliers	100387	1117 (5.40-3.60)
Sidechain outliers	100360	1099 (5.40-3.60)
RSRZ outliers	91569	1075 (5.40-3.60)

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  $\geq 3$ , 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	G	481	<div> <div>76%</div> <div>14%</div> <div>• 8%</div> </div>
2	B	153	<div> <div>%</div> <div>72%</div> <div>8%</div> <div>20%</div> </div>
3	L	214	<div> <div>78%</div> <div>18%</div> <div>• • •</div> </div>
4	H	236	<div> <div>2%</div> <div>61%</div> <div>33%</div> <div>• 5%</div> </div>
5	D	240	<div> <div>93%</div> <div>8%</div> </div>
6	E	216	<div> <div>94%</div> <div>5%</div> <div>•</div> </div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11836 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 gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	442	Total	C	N	O	S	0	0	0
			3483	2202	608	646	27			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	106	GLU	THR	conflict	UNP Q2N0S6
G	134	TYR	VAL	conflict	UNP Q2N0S6
G	135	ALA	THR	conflict	UNP Q2N0S6
G	136	PRO	ASN	conflict	UNP Q2N0S6
G	137	PHE	ASN	conflict	UNP Q2N0S6
G	138	LEU	ILE	conflict	UNP Q2N0S6
G	139	ILE	THR	conflict	UNP Q2N0S6
G	140	ASN	ASP	conflict	UNP Q2N0S6
G	149	ASN	ASP	conflict	UNP Q2N0S6
G	271	ILE	MET	conflict	UNP Q2N0S6
G	288	LEU	PHE	conflict	UNP Q2N0S6
G	304	VAL	ARG	conflict	UNP Q2N0S6
G	319	TYR	ALA	conflict	UNP Q2N0S6
G	328	MET	GLN	conflict	UNP Q2N0S6
G	332	ASN	THR	conflict	UNP Q2N0S6
G	363	GLN	ASN	conflict	UNP Q2N0S6
G	501	CYS	ALA	conflict	UNP Q2N0S6
G	509	ARG	-	expression tag	UNP Q2N0S6
G	510	ARG	-	expression tag	UNP Q2N0S6
G	511	ARG	-	expression tag	UNP Q2N0S6
G	512	ARG	-	expression tag	UNP Q2N0S6
G	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	122	Total	C	N	O	S	0	0	0
			963	605	166	186	6			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	519	SER	PHE	conflict	UNP Q2N0S6
B	559	PRO	ILE	conflict	UNP Q2N0S6
B	561	PRO	ALA	conflict	UNP Q2N0S6
B	568	ASP	LEU	conflict	UNP Q2N0S6
B	570	HIS	VAL	conflict	UNP Q2N0S6
B	585	HIS	ARG	conflict	UNP Q2N0S6
B	605	CYS	THR	conflict	UNP Q2N0S6

- Molecule 3 is a protein called Fab PGT124 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	210	Total	C	N	O	S	0	0	0
			1595	1005	270	315	5			

- Molecule 4 is a protein called Fab PGT124 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	225	Total	C	N	O	S	0	0	0
			1714	1090	286	333	5			

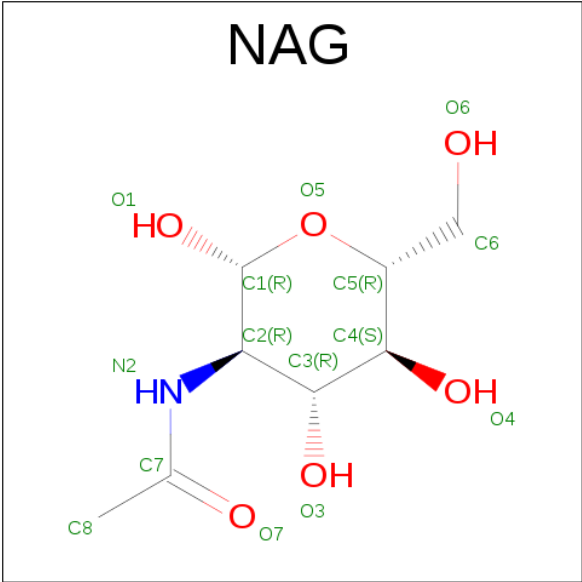
- Molecule 5 is a protein called Fab 35022 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	240	Total	C	N	O	S	0	0	0
			1813	1150	303	352	8			

- Molecule 6 is a protein called Fab 35022 light chain.

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

- Molecule 7 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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		

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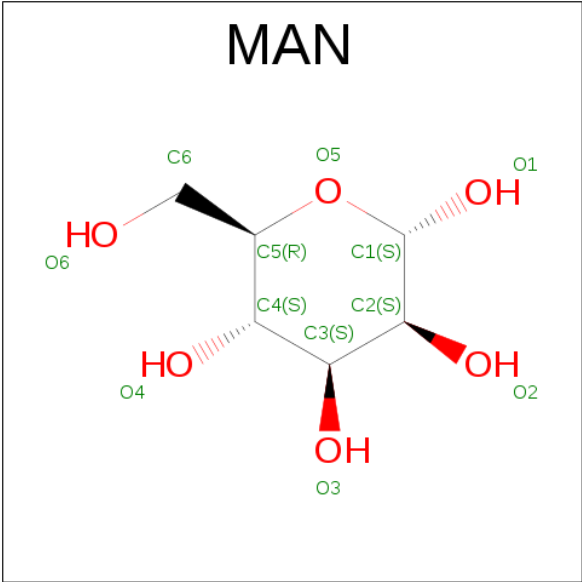
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1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

- Molecule 8 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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		

- Molecule 9 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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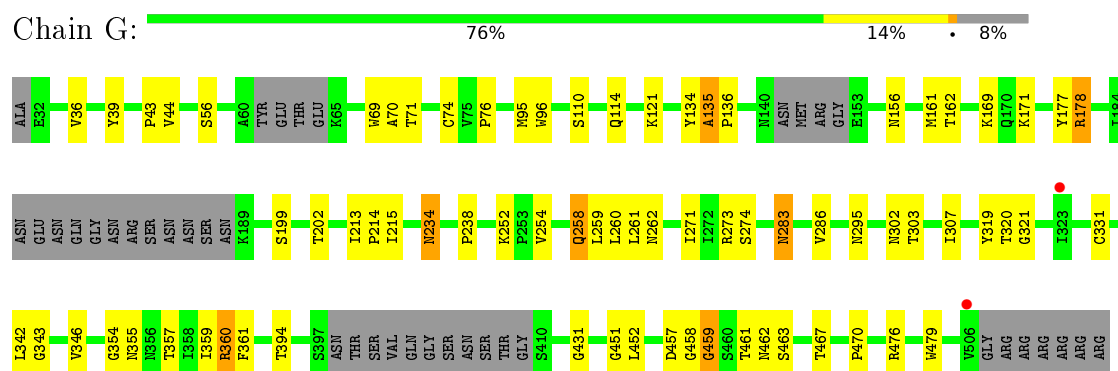
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		

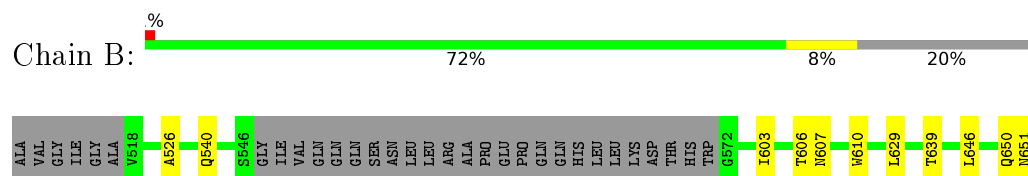
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

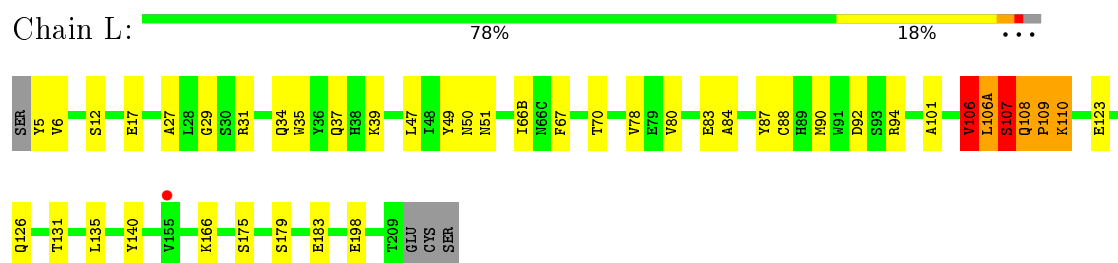
#### • Molecule 1: Envelope glycoprotein gp160



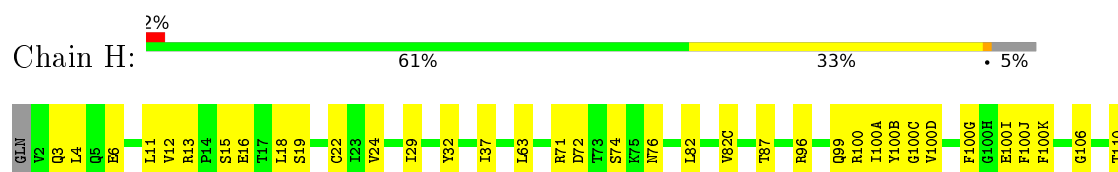
#### • Molecule 2: Envelope glycoprotein gp160

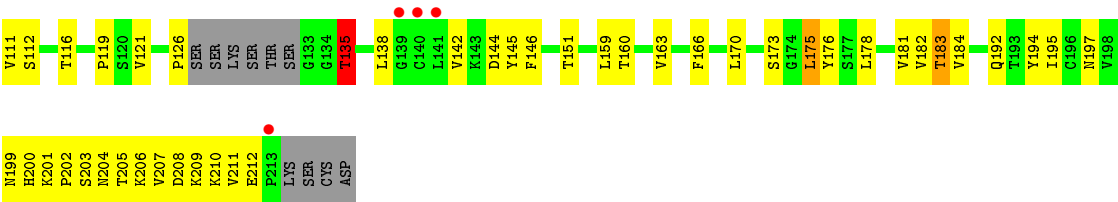


#### • Molecule 3: Fab PGT124 light chain

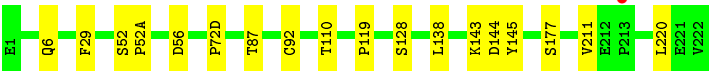
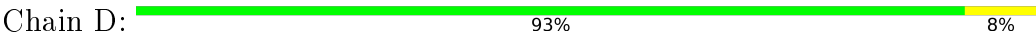


#### • Molecule 4: Fab PGT124 heavy chain

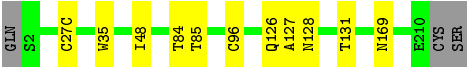




• Molecule 5: Fab 35022 heavy chain



• Molecule 6: Fab 35022 light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.92Å 127.92Å 313.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.01 – 4.50 49.58 – 4.49	Depositor EDS
% Data completeness (in resolution range)	98.4 (50.01-4.50) 98.3 (49.58-4.49)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 4.45Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.270 , 0.309 0.271 , 0.303	Depositor DCC
$R_{free}$ test set	844 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	105.6	Xtriage
Anisotropy	0.753	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 103.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.137 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	11836	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	187.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	G	0.59	0/3557	0.78	4/4829 (0.1%)
2	B	0.58	0/979	0.73	0/1327
3	L	0.74	1/1638 (0.1%)	0.84	2/2238 (0.1%)
4	H	0.76	1/1757 (0.1%)	0.84	1/2399 (0.0%)
5	D	0.37	0/1860	0.56	0/2533
6	E	0.40	0/1659	0.58	0/2269
All	All	0.59	2/11450 (0.0%)	0.74	7/15595 (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
1	G	0	3
3	L	0	1
6	E	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	106	VAL	C-N	-5.84	1.20	1.34
4	H	135	THR	N-CA	-5.27	1.35	1.46

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	355	ASN	N-CA-C	7.29	130.67	111.00
1	G	177	TYR	N-CA-C	-7.01	92.08	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	106	VAL	O-C-N	-6.71	111.97	122.70
1	G	234	ASN	N-CA-C	-6.32	93.95	111.00
1	G	459	GLY	N-CA-C	-5.94	98.25	113.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	E	27(C)	CYS	Peptide
1	G	178	ARG	Mainchain
1	G	234	ASN	Mainchain,Peptide
3	L	106	VAL	Mainchain

## 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	G	3483	0	3440	41	0
2	B	963	0	936	11	0
3	L	1595	0	1540	36	0
4	H	1714	0	1681	94	0
5	D	1813	0	1784	10	0
6	E	1615	0	1544	4	0
7	B	42	0	39	0	0
7	G	336	0	296	2	0
8	G	66	0	51	0	0
9	G	209	0	180	1	0
All	All	11836	0	11491	188	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 8.

The worst 5 of 188 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:L:83:GLU:CG	3:L:106:VAL:HG23	1.78	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:108:GLN:HB3	3:L:140:TYR:CE1	1.88	1.07
3:L:83:GLU:HG2	3:L:106:VAL:HG23	1.42	0.99
4:H:121:VAL:O	4:H:209:LYS:HE3	1.65	0.96
4:H:119:PRO:HD2	4:H:205:THR:HG21	1.46	0.95

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	G	432/481 (90%)	406 (94%)	23 (5%)	3 (1%)	26	71
2	B	118/153 (77%)	113 (96%)	5 (4%)	0	100	100
3	L	208/214 (97%)	203 (98%)	4 (2%)	1 (0%)	34	77
4	H	221/236 (94%)	212 (96%)	9 (4%)	0	100	100
5	D	238/240 (99%)	234 (98%)	4 (2%)	0	100	100
6	E	211/216 (98%)	206 (98%)	5 (2%)	0	100	100
All	All	1428/1540 (93%)	1374 (96%)	50 (4%)	4 (0%)	46	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	135	ALA
1	G	136	PRO
1	G	354	GLY
3	L	109	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	G	395/428 (92%)	385 (98%)	10 (2%)	55	82
2	B	105/130 (81%)	103 (98%)	2 (2%)	65	86
3	L	176/180 (98%)	167 (95%)	9 (5%)	29	67
4	H	193/204 (95%)	186 (96%)	7 (4%)	42	75
5	D	203/203 (100%)	203 (100%)	0	100	100
6	E	186/189 (98%)	183 (98%)	3 (2%)	70	88
All	All	1258/1334 (94%)	1227 (98%)	31 (2%)	55	82

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	106	VAL
3	L	108	GLN
6	E	96	CYS
3	L	106(A)	LEU
3	L	110	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	L	51	ASN
3	L	108	GLN
4	H	192	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 ⓘ

52 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	2	14,14,15	0.40	0	15,19,21	0.74	1 (6%)
7	NAG	B	702	2	14,14,15	0.37	0	15,19,21	1.00	1 (6%)
7	NAG	B	703	2	14,14,15	0.40	0	15,19,21	0.76	0
7	NAG	G	601	1,7	14,14,15	0.36	0	15,19,21	0.79	0
7	NAG	G	602	8,7	14,14,15	0.35	0	15,19,21	0.82	0
8	BMA	G	603	9,7	11,11,12	0.33	0	15,15,17	0.74	0
9	MAN	G	604	8	11,11,12	0.28	0	15,15,17	0.79	0
9	MAN	G	605	9,8	11,11,12	0.29	0	15,15,17	0.78	0
9	MAN	G	606	9	11,11,12	0.26	0	15,15,17	0.91	1 (6%)
9	MAN	G	607	9	11,11,12	0.25	0	15,15,17	0.68	0
7	NAG	G	608	1,7	14,14,15	0.32	0	15,19,21	0.80	1 (6%)
7	NAG	G	609	7	14,14,15	0.27	0	15,19,21	0.53	0
7	NAG	G	610	1	14,14,15	0.45	0	15,19,21	0.72	0
7	NAG	G	611	1	14,14,15	0.30	0	15,19,21	0.71	0
7	NAG	G	612	1,7	14,14,15	0.33	0	15,19,21	0.87	0
7	NAG	G	613	7	14,14,15	0.29	0	15,19,21	1.24	1 (6%)
7	NAG	G	614	1,7	14,14,15	0.37	0	15,19,21	0.78	0
7	NAG	G	615	7	14,14,15	0.36	0	15,19,21	0.92	1 (6%)
7	NAG	G	616	1,7	14,14,15	0.28	0	15,19,21	0.68	0
7	NAG	G	617	7	14,14,15	0.29	0	15,19,21	0.89	0
7	NAG	G	618	1,7	14,14,15	0.39	0	15,19,21	1.03	1 (6%)
7	NAG	G	619	8,7	14,14,15	0.33	0	15,19,21	0.62	0
8	BMA	G	620	9,7	11,11,12	0.42	0	15,15,17	0.67	0
9	MAN	G	621	9,8	11,11,12	0.41	0	15,15,17	0.90	1 (6%)
9	MAN	G	622	9	11,11,12	0.27	0	15,15,17	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	G	623	1,7	14,14,15	0.33	0	15,19,21	1.06	1 (6%)
7	NAG	G	624	8,7	14,14,15	0.24	0	15,19,21	0.67	0
8	BMA	G	625	9,7	11,11,12	0.35	0	15,15,17	0.56	0
9	MAN	G	626	8	11,11,12	0.24	0	15,15,17	0.80	1 (6%)
7	NAG	G	627	1,7	14,14,15	0.25	0	15,19,21	0.87	0
7	NAG	G	628	8,7	14,14,15	0.28	0	15,19,21	1.26	1 (6%)
8	BMA	G	629	9,7	11,11,12	0.28	0	15,15,17	0.60	0
9	MAN	G	630	8	11,11,12	0.28	0	15,15,17	0.72	1 (6%)
7	NAG	G	631	1,7	14,14,15	0.25	0	15,19,21	0.53	0
7	NAG	G	632	8,7	14,14,15	0.55	0	15,19,21	1.73	3 (20%)
8	BMA	G	633	9,7	11,11,12	0.54	0	15,15,17	1.36	2 (13%)
9	MAN	G	634	8	11,11,12	0.25	0	15,15,17	0.68	0
9	MAN	G	635	9,8	11,11,12	0.34	0	15,15,17	1.17	1 (6%)
9	MAN	G	636	9	11,11,12	0.34	0	15,15,17	0.81	0
9	MAN	G	637	9	11,11,12	0.30	0	15,15,17	0.81	1 (6%)
7	NAG	G	638	1,7	14,14,15	0.46	0	15,19,21	1.07	1 (6%)
7	NAG	G	639	8,7	14,14,15	0.34	0	15,19,21	0.87	0
8	BMA	G	640	9,7	11,11,12	0.38	0	15,15,17	1.05	1 (6%)
9	MAN	G	641	9,8	11,11,12	0.46	0	15,15,17	1.02	0
9	MAN	G	642	9	11,11,12	0.25	0	15,15,17	0.75	0
9	MAN	G	643	9	11,11,12	0.38	0	15,15,17	0.85	1 (6%)
9	MAN	G	644	9,8	11,11,12	0.50	0	15,15,17	1.66	3 (20%)
9	MAN	G	645	9	11,11,12	0.28	0	15,15,17	1.09	1 (6%)
9	MAN	G	646	9	11,11,12	0.33	0	15,15,17	0.81	0
9	MAN	G	647	9	11,11,12	0.32	0	15,15,17	0.50	0
7	NAG	G	648	1	14,14,15	0.43	0	15,19,21	0.71	0
7	NAG	G	649	1	14,14,15	0.35	0	15,19,21	0.54	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	2	-	0/6/23/26	0/1/1/1
7	NAG	B	702	2	-	0/6/23/26	0/1/1/1
7	NAG	B	703	2	-	0/6/23/26	0/1/1/1
7	NAG	G	601	1,7	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
9	MAN	G	607	9	-	0/2/19/22	0/1/1/1
7	NAG	G	608	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	609	7	-	0/6/23/26	0/1/1/1
7	NAG	G	610	1	-	0/6/23/26	0/1/1/1
7	NAG	G	611	1	-	0/6/23/26	0/1/1/1
7	NAG	G	612	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	613	7	-	0/6/23/26	0/1/1/1
7	NAG	G	614	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	615	7	-	0/6/23/26	0/1/1/1
7	NAG	G	616	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	617	7	-	0/6/23/26	0/1/1/1
7	NAG	G	618	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	619	8,7	-	0/6/23/26	0/1/1/1
8	BMA	G	620	9,7	-	0/2/19/22	0/1/1/1
9	MAN	G	621	9,8	-	0/2/19/22	0/1/1/1
9	MAN	G	622	9	-	0/2/19/22	0/1/1/1
7	NAG	G	623	1,7	-	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
7	NAG	G	627	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	628	8,7	-	0/6/23/26	0/1/1/1
8	BMA	G	629	9,7	-	0/2/19/22	0/1/1/1
9	MAN	G	630	8	-	0/2/19/22	0/1/1/1
7	NAG	G	631	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	632	8,7	-	0/6/23/26	0/1/1/1
8	BMA	G	633	9,7	-	0/2/19/22	0/1/1/1
9	MAN	G	634	8	-	0/2/19/22	0/1/1/1
9	MAN	G	635	9,8	-	0/2/19/22	0/1/1/1
9	MAN	G	636	9	-	0/2/19/22	0/1/1/1
9	MAN	G	637	9	-	0/2/19/22	0/1/1/1
7	NAG	G	638	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	639	8,7	-	0/6/23/26	0/1/1/1
8	BMA	G	640	9,7	-	0/2/19/22	0/1/1/1
9	MAN	G	641	9,8	-	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
9	MAN	G	644	9,8	-	0/2/19/22	0/1/1/1
9	MAN	G	645	9	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MAN	G	646	9	-	0/2/19/22	0/1/1/1
9	MAN	G	647	9	-	0/2/19/22	0/1/1/1
7	NAG	G	648	1	-	0/6/23/26	0/1/1/1
7	NAG	G	649	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	633	BMA	O5-C5-C4	-2.77	105.55	110.13
7	G	623	NAG	O5-C5-C4	-2.69	105.69	110.13
8	G	640	BMA	O3-C3-C2	-2.58	105.29	110.01
7	G	632	NAG	O7-C7-C8	-2.52	117.43	122.07
9	G	645	MAN	O5-C5-C4	-2.16	106.56	110.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	610	NAG	1	0
7	G	639	NAG	1	0
9	G	643	MAN	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	G	442/481 (91%)	-0.28	2 (0%) 91 88	86, 148, 210, 294	0
2	B	122/153 (79%)	-0.27	1 (0%) 87 82	94, 147, 226, 290	0
3	L	210/214 (98%)	-0.43	1 (0%) 91 88	123, 197, 243, 308	0
4	H	225/236 (95%)	-0.20	4 (1%) 71 62	126, 193, 269, 333	0
5	D	240/240 (100%)	-0.26	1 (0%) 93 90	118, 219, 342, 435	0
6	E	213/216 (98%)	-0.44	0 100 100	133, 211, 303, 336	0
All	All	1452/1540 (94%)	-0.31	9 (0%) 90 86	86, 180, 288, 435	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	664	ASP	4.3
5	D	213	PRO	4.3
4	H	140	CYS	3.3
4	H	213	PRO	2.8
4	H	141	LEU	2.6

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
9	MAN	G	637	11/12	0.88	0.33	1.91	201,222,227,240	0
7	NAG	B	702	14/15	0.77	0.21	0.89	181,246,258,264	0
7	NAG	B	703	14/15	0.73	0.23	0.51	182,210,231,246	0
7	NAG	G	638	14/15	0.92	0.24	0.26	145,147,164,165	0
7	NAG	G	601	14/15	0.92	0.26	-0.29	95,123,138,142	0
7	NAG	G	616	14/15	0.89	0.21	-0.42	182,193,207,223	0
7	NAG	G	612	14/15	0.90	0.19	-0.80	128,139,149,153	0
9	MAN	G	645	11/12	0.91	0.16	-0.80	140,149,154,158	0
8	BMA	G	633	11/12	0.95	0.13	-0.91	172,190,217,226	0
9	MAN	G	644	11/12	0.96	0.16	-1.05	124,138,150,160	0
7	NAG	G	632	14/15	0.91	0.15	-1.18	127,153,170,185	0
7	NAG	G	639	14/15	0.93	0.19	-1.25	124,153,163,167	0
7	NAG	G	631	14/15	0.96	0.16	-2.30	120,145,154,158	0
7	NAG	G	627	14/15	0.86	0.44	-	172,183,221,226	0
7	NAG	G	648	14/15	0.84	0.22	-	194,218,233,242	0
7	NAG	G	615	14/15	0.78	0.26	-	175,190,195,197	0
8	BMA	G	603	11/12	0.93	0.18	-	175,180,187,191	0
9	MAN	G	622	11/12	0.88	0.20	-	250,253,264,267	0
7	NAG	G	609	14/15	0.87	0.26	-	177,195,204,211	0
8	BMA	G	625	11/12	0.75	0.34	-	269,290,301,304	0
9	MAN	G	646	11/12	0.94	0.17	-	136,146,152,163	0
7	NAG	G	623	14/15	0.92	0.23	-	169,184,188,192	0
9	MAN	G	635	11/12	0.76	0.29	-	233,241,266,269	0
7	NAG	G	628	14/15	0.90	0.36	-	178,204,243,283	0
9	MAN	G	604	11/12	0.89	0.31	-	196,202,207,212	0
7	NAG	B	701	14/15	0.86	0.28	-	180,195,197,202	0
8	BMA	G	620	11/12	0.82	0.22	-	211,250,287,290	0
9	MAN	G	605	11/12	0.88	0.21	-	180,196,201,220	0
9	MAN	G	607	11/12	0.81	0.25	-	271,282,291,295	0
9	MAN	G	647	11/12	0.95	0.16	-	186,193,203,211	0
9	MAN	G	606	11/12	0.85	0.24	-	213,227,236,253	0
7	NAG	G	611	14/15	0.86	0.30	-	198,215,240,240	0
9	MAN	G	634	11/12	0.90	0.15	-	183,194,203,218	0
7	NAG	G	602	14/15	0.96	0.19	-	153,160,170,180	0
8	BMA	G	629	11/12	0.59	0.29	-	292,308,315,324	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
9	MAN	G	630	11/12	0.50	0.38	-	262,304,313,326	0
7	NAG	G	610	14/15	0.74	0.30	-	190,195,211,212	0
9	MAN	G	621	11/12	0.81	0.28	-	272,282,290,298	0
7	NAG	G	617	14/15	0.74	0.33	-	204,228,238,240	0
7	NAG	G	618	14/15	0.93	0.21	-	144,157,177,185	0
9	MAN	G	642	11/12	0.96	0.14	-	164,173,179,193	0
7	NAG	G	614	14/15	0.94	0.19	-	136,150,161,170	0
9	MAN	G	636	11/12	0.83	0.32	-	244,257,266,268	0
7	NAG	G	649	14/15	0.69	0.23	-	206,220,224,233	0
9	MAN	G	641	11/12	0.91	0.17	-	174,187,200,213	0
7	NAG	G	608	14/15	0.92	0.20	-	171,175,181,192	0
9	MAN	G	626	11/12	0.88	0.23	-	226,238,250,252	0
7	NAG	G	624	14/15	0.92	0.22	-	186,216,231,247	0
7	NAG	G	619	14/15	0.91	0.27	-	186,205,231,233	0
7	NAG	G	613	14/15	0.92	0.18	-	149,163,173,185	0
9	MAN	G	643	11/12	0.80	0.22	-	216,224,236,242	0
8	BMA	G	640	11/12	0.94	0.17	-	141,147,156,166	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.