



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:14 PM GMT

PDB ID : 4BXS  
Title : Crystal Structure of the Prothrombinase Complex from the Venom of Pseudonaja Textilis  
Authors : Lechtenberg, B.C.; Murray-Rust, T.A.; Johnson, D.J.D.; Adams, T.E.; Krishnaswamy, S.; Camire, R.M.; Huntington, J.A.  
Deposited on : 2013-07-15  
Resolution : 3.32 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

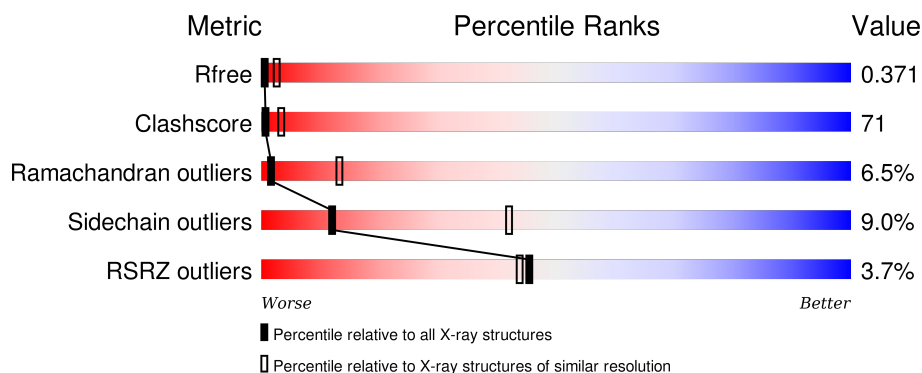
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.32 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	1198 (3.40-3.24)
Clashscore	102246	1280 (3.40-3.24)
Ramachandran outliers	100387	1260 (3.40-3.24)
Sidechain outliers	100360	1259 (3.40-3.24)
RSRZ outliers	91569	1203 (3.40-3.24)

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	A	423	
2	V	1430	

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
3	FUC	V	1433	X	-	-	-
5	NAG	V	1519	X	-	-	-
6	NAG	V	1521	X	-	-	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11295 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 FACTOR X-LIKE PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			1587	981	290	298	18			

- Molecule 2 is a protein called VENOM PROTHROMBIN ACTIVATOR PSEUTARIN-C NON-CATALYTIC SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	V	1262	Total	C	N	O	S	64	0	0
			9408	6020	1587	1766	35			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	50	LYS	GLU	CONFLICT	UNP Q7SZN0
V	1287	LYS	SER	CONFLICT	UNP Q7SZN0
V	1305	PHE	SER	CONFLICT	UNP Q7SZN0

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	V	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 4 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	V	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	V	2	Total	C	N	O	0	0
			25	14	2	9		
5	V	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	V	2	Total	Ca	0	0
			2	2		

- Molecule 8 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	V	1	Total	Cu	0	0
			1	1		

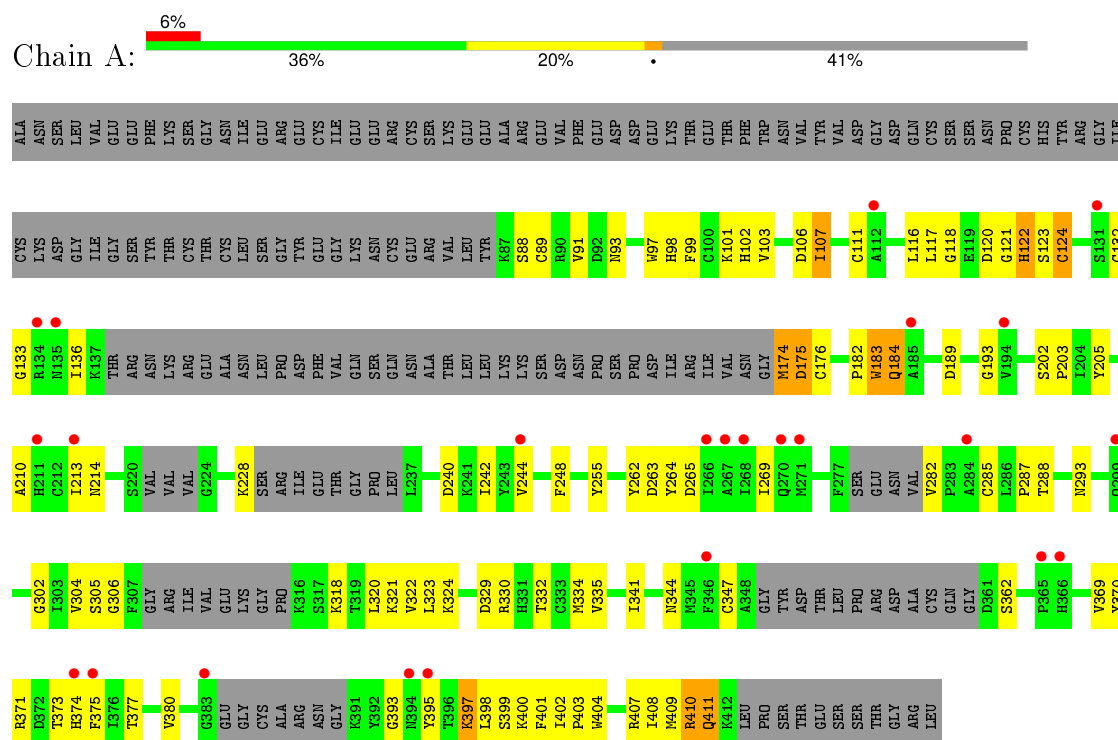
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	7	Total 7	O 7	0	0
9	V	105	Total 105	O 105	0	0

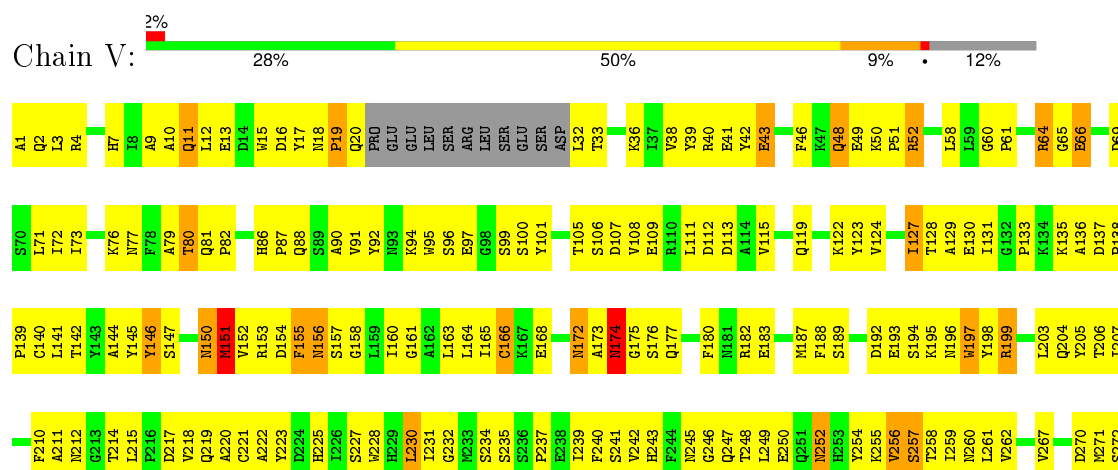
### 3 Residue-property plots

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: FACTOR X-LIKE PROTEASE



#### • Molecule 2: VENOM PROTHROMBIN ACTIVATOR PSEUTARIN-C NON-CATALYTIC SUB-UNIT









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.31Å 115.31Å 429.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.81 – 3.32 89.81 – 3.32	Depositor EDS
% Data completeness (in resolution range)	99.1 (89.81-3.32) 99.1 (89.81-3.32)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.298 , 0.368 0.289 , 0.371	Depositor DCC
$R_{free}$ test set	2262 reflections (5.46%)	DCC
Wilson B-factor (Å <sup>2</sup> )	86.3	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 116.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	3 of 43728 reflections (0.007%)	Xtriage
$F_o, F_c$ correlation	0.81	EDS
Total number of atoms	11295	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, CA, FUC, CU, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.20	0/1617	0.39	0/2210
2	V	0.23	0/9671	0.43	4/13230 (0.0%)
All	All	0.22	0/11288	0.43	4/15440 (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
2	V	0	5
3	V	1	0
5	V	1	0
All	All	2	5

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	670	ASP	O-C-N	-12.35	102.94	122.70
2	V	657	TYR	O-C-N	-6.42	112.42	122.70
2	V	670	ASP	C-N-CA	6.42	137.75	121.70
2	V	657	TYR	C-N-CA	5.43	135.28	121.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	V	1433	FUC	C1
5	V	1519	NAG	C1

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	V	657	TYR	Peptide
2	V	658	ASP	Peptide
2	V	668	GLU	Peptide
2	V	669	GLU	Peptide
2	V	670	ASP	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	A	1587	0	1171	118	0
2	V	9408	0	8230	1343	0
3	V	24	0	22	4	0
4	V	94	0	79	11	0
5	V	53	0	46	3	0
6	V	14	0	13	3	0
7	V	2	0	0	0	0
8	V	1	0	0	0	0
9	A	7	0	0	0	0
9	V	105	0	0	19	0
All	All	11295	0	9561	1458	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 71.

The worst 5 of 1458 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:V:337:ALA:HB3	2:V:362:LYS:CD	1.25	1.60
2:V:337:ALA:CB	2:V:362:LYS:HD3	1.11	1.55
2:V:1205:SER:CB	2:V:1211:TRP:HB3	1.32	1.55
2:V:1094:LEU:HD23	2:V:1110:PHE:CD1	1.36	1.53
2:V:1309:LEU:HD12	2:V:1423:GLU:CB	1.33	1.52

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	232/423 (55%)	195 (84%)	27 (12%)	10 (4%)	3	24
2	V	1243/1430 (87%)	961 (77%)	196 (16%)	86 (7%)	1	12
All	All	1475/1853 (80%)	1156 (78%)	223 (15%)	96 (6%)	1	13

5 of 96 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	ILE
1	A	305	SER
1	A	410	ARG
2	V	52	ARG
2	V	66	GLU

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	111/368 (30%)	106 (96%)	5 (4%)	34	71
2	V	878/1260 (70%)	794 (90%)	84 (10%)	10	38
All	All	989/1628 (61%)	900 (91%)	89 (9%)	12	42

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	V	877	ARG

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Mol	Chain	Res	Type
2	V	1030	MET
2	V	1364	THR
2	V	926	ARG
2	V	984	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
2	V	602	HIS
2	V	1037	HIS
2	V	1319	GLN
2	V	922	GLN
2	V	1055	HIS

### 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 ⓘ

14 carbohydrates 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	$\# Z  > 2$
3	NAG	V	1432	3,2	14,14,15	0.78	0	15,19,21	1.01	2 (13%)
3	FUC	V	1433	3	10,10,11	0.63	0	14,14,16	0.80	0
4	MAN	V	1501	4	11,11,12	0.61	0	14,15,17	0.59	0
4	BMA	V	1502	4	11,11,12	0.30	0	14,15,17	0.76	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	V	1508	4	14,14,15	0.53	0	15,19,21	0.72	0
4	NAG	V	1509	2,4	14,14,15	0.49	0	15,19,21	0.84	0
4	MAN	V	1511	4	11,11,12	0.66	0	14,15,17	0.76	0
4	MAN	V	1512	4	11,11,12	0.60	0	14,15,17	0.88	1 (7%)
4	MAN	V	1513	4	11,11,12	0.63	0	14,15,17	0.62	0
4	MAN	V	1514	4	11,11,12	0.68	0	14,15,17	0.79	0
5	NAG	V	1515	2,5	14,14,15	0.55	0	15,19,21	0.70	0
5	NAG	V	1516	5	11,11,15	0.61	0	13,15,21	0.67	0
5	NAG	V	1519	2,5	14,14,15	0.59	0	15,19,21	0.71	0
5	NAG	V	1520	5	14,14,15	0.53	0	15,19,21	0.66	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
3	NAG	V	1432	3,2	-	0/6/23/26	0/1/1/1
3	FUC	V	1433	3	1/1/4/5	0/0/17/20	0/1/1/1
4	MAN	V	1501	4	-	0/2/19/22	0/1/1/1
4	BMA	V	1502	4	-	0/2/19/22	0/1/1/1
4	NAG	V	1508	4	-	0/6/23/26	0/1/1/1
4	NAG	V	1509	2,4	-	0/6/23/26	0/1/1/1
4	MAN	V	1511	4	-	0/2/19/22	0/1/1/1
4	MAN	V	1512	4	-	0/2/19/22	0/1/1/1
4	MAN	V	1513	4	-	0/2/19/22	0/1/1/1
4	MAN	V	1514	4	-	0/2/19/22	0/1/1/1
5	NAG	V	1515	2,5	-	0/6/23/26	0/1/1/1
5	NAG	V	1516	5	-	0/2/19/26	0/1/1/1
5	NAG	V	1519	2,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	V	1520	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	1512	MAN	C1-C2-C3	-2.11	107.05	109.54
3	V	1432	NAG	C2-N2-C7	2.15	125.80	123.04
4	V	1502	BMA	C1-C2-C3	2.37	112.34	109.54
3	V	1432	NAG	C4-C3-C2	2.40	114.96	111.23

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	V	1519	NAG	C1
3	V	1433	FUC	C1

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	V	1432	NAG	4	0
4	V	1501	MAN	2	0
4	V	1502	BMA	2	0
4	V	1508	NAG	3	0
4	V	1509	NAG	5	0
4	V	1512	MAN	1	0
4	V	1513	MAN	1	0
5	V	1519	NAG	1	0
5	V	1520	NAG	2	0

## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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	NAG	V	1521	2	14,14,15	0.51	0	15,19,21	0.66	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
6	NAG	V	1521	2	1/1/5/7	0/6/23/26	0/1/1/1

There are no bond length outliers.



There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	V	1521	NAG	C1

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	V	1521	NAG	3	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	A	248/423 (58%)	0.33	24 (9%) 10 11	82, 154, 205, 249	0
2	V	1249/1430 (87%)	0.08	31 (2%) 61 60	65, 122, 172, 255	0
All	All	1497/1853 (80%)	0.12	55 (3%) 45 44	65, 126, 185, 255	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	375	PHE	5.0
2	V	1263	ILE	4.9
2	V	1188	THR	4.5
1	A	366	HIS	3.9
2	V	1201	PHE	3.8

### 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](#)

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
4	NAG	V	1509	14/15	0.96	0.17	-0.84	109,122,134,138	0
4	NAG	V	1508	14/15	0.96	0.18	-0.96	100,114,135,135	0
4	MAN	V	1501	11/12	0.93	0.21	-	122,131,153,163	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	V	1516	11/15	0.88	0.41	-	171,180,203,215	0
4	MAN	V	1512	11/12	0.93	0.16	-	89,146,182,203	0
5	NAG	V	1519	14/15	0.82	0.13	-	132,201,219,237	0
5	NAG	V	1520	14/15	0.77	0.15	-	166,195,234,249	0
4	MAN	V	1513	11/12	0.86	0.34	-	166,216,232,241	0
4	BMA	V	1502	11/12	0.95	0.15	-	120,126,151,159	0
5	NAG	V	1515	14/15	0.92	0.27	-	123,145,212,220	0
3	FUC	V	1433	10/11	0.83	0.15	-	174,220,248,281	0
4	MAN	V	1514	11/12	0.87	0.29	-	99,147,176,234	0
3	NAG	V	1432	14/15	0.86	0.10	-	170,211,254,267	0
4	MAN	V	1511	11/12	0.95	0.24	-	124,154,178,181	0

## 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. 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( $\text{\AA}^2$ )	Q<0.9
7	CA	V	2431	1/1	0.99	0.08	-1.23	105,105,105,105	0
7	CA	V	2430	1/1	0.99	0.12	-1.26	88,88,88,88	0
8	CU	V	2432	1/1	0.98	0.11	-3.11	124,124,124,124	0
6	NAG	V	1521	14/15	0.81	0.32	-	152,206,263,286	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.