



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 30, 2017 – 06:39 PM EST

PDB ID : 3DGV  
Title : Crystal structure of thrombin activatable fibrinolysis inhibitor (TAFI)  
Authors : Anand, K.; Pallares, I.; Valnickova, Z.; Christensen, T.; Schreuder, H.; Enghild, J.  
Deposited on : 2008-06-16  
Resolution : 2.50 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-20028442
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-20028442

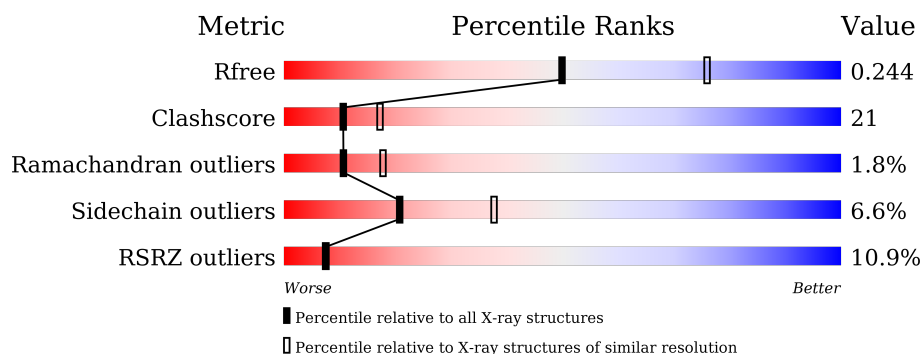
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	401	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>25%</div> <div>.</div> </div> </div>
1	B	401	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>29%</div> <div>.</div> </div> </div>
1	C	401	<div> <div>28%</div> <div> <div></div> <div>37%</div> <div>51%</div> <div>7%</div> <div>5%</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
11	MLI	A	328	-	-	-	X
11	MLI	B	329	-	-	-	X
4	NAG	A	313	-	-	-	X
4	NAG	B	314	-	-	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 11015 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 Carboxypeptidase B2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3278	2097	565	600	16			
1	B	401	Total	C	N	O	S	0	0	0
			3275	2094	564	601	16			
1	C	379	Total	C	N	O	S	0	0	0
			3068	1958	525	569	16			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		

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

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

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		

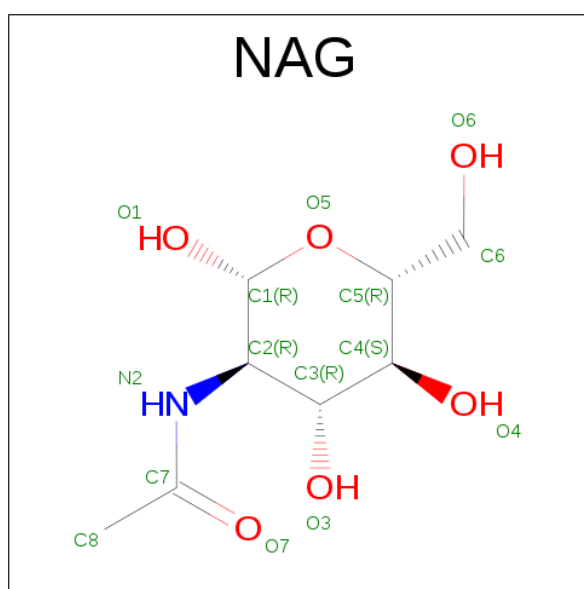
- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

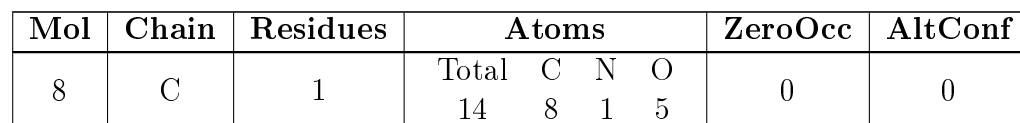
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 is SUGAR (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		

- Molecule 8 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula:  $C_8H_{15}NO_6$ ).



- | Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 9   | B     | 1        | Total Zn<br>1 1 | 0       | 0       |
| 9   | A     | 1        | Total Zn<br>1 1 | 0       | 0       |
| 9   | C     | 1        | Total Zn<br>1 1 | 0       | 0       |

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



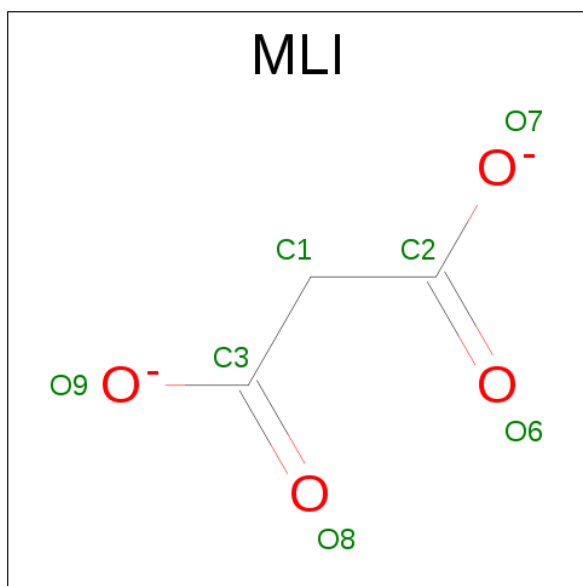
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	B	1	Total	O	S	0	0
			5	4	1		
10	B	1	Total	O	S	0	0
			5	4	1		
10	B	1	Total	O	S	0	0
			5	4	1		
10	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	O	S	0	0
			5	4	1		
10	B	1	Total	O	S	0	0
			5	4	1		
10	B	1	Total	O	S	0	0
			5	4	1		
10	B	1	Total	O	S	0	0
			5	4	1		
10	B	1	Total	O	S	0	0
			5	4	1		
10	C	1	Total	O	S	0	0
			5	4	1		
10	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 11 is MALONATE ION (three-letter code: MLI) (formula:  $\text{C}_3\text{H}_2\text{O}_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			7	3	4		
11	B	1	Total	C	O	0	0
			7	3	4		
11	C	1	Total	C	O	0	0
			7	3	4		



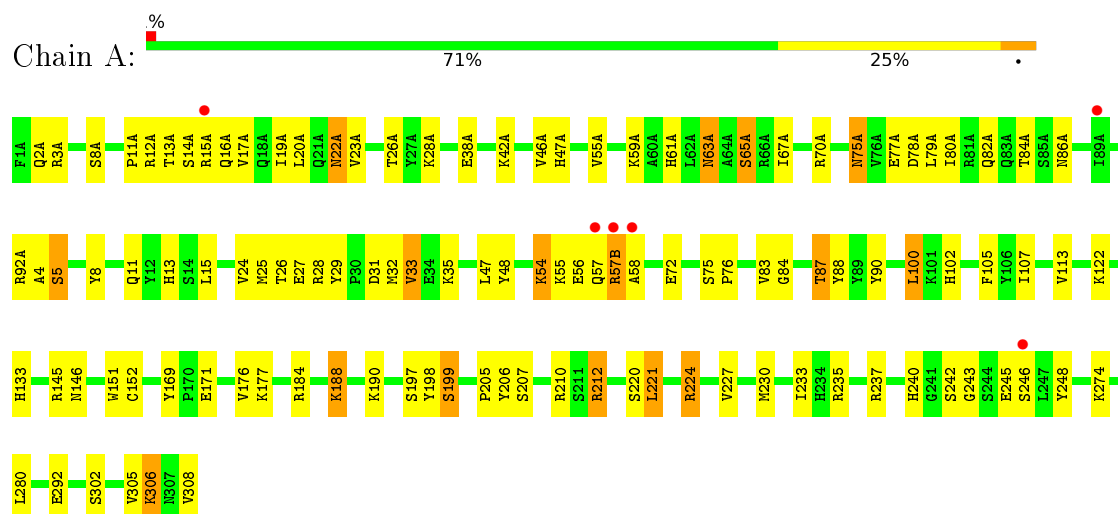
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	484	Total 484	O 484	0	0
12	B	417	Total 417	O 417	0	0
12	C	118	Total 118	O 118	0	0

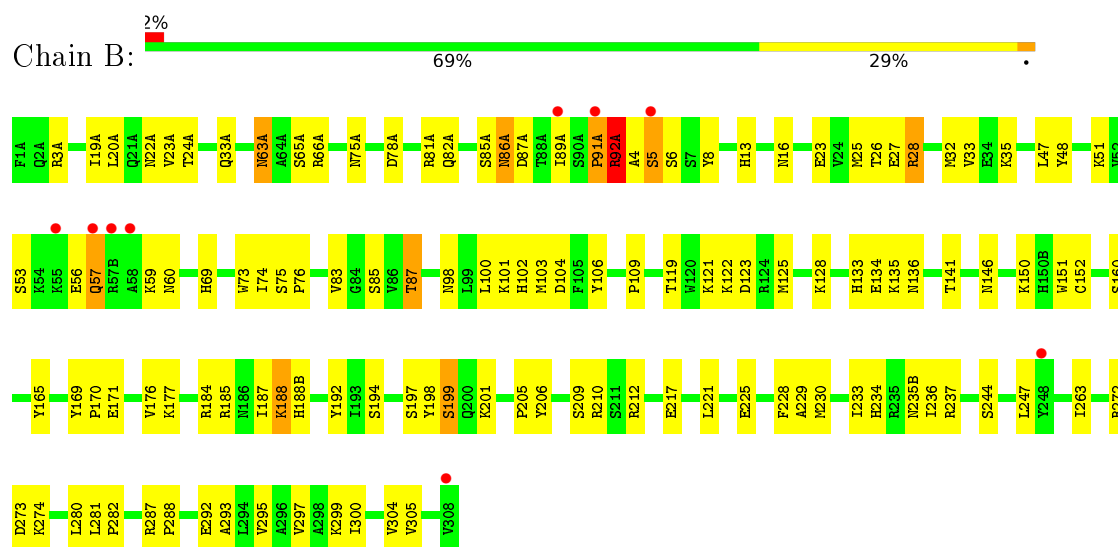
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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: Carboxypeptidase B2

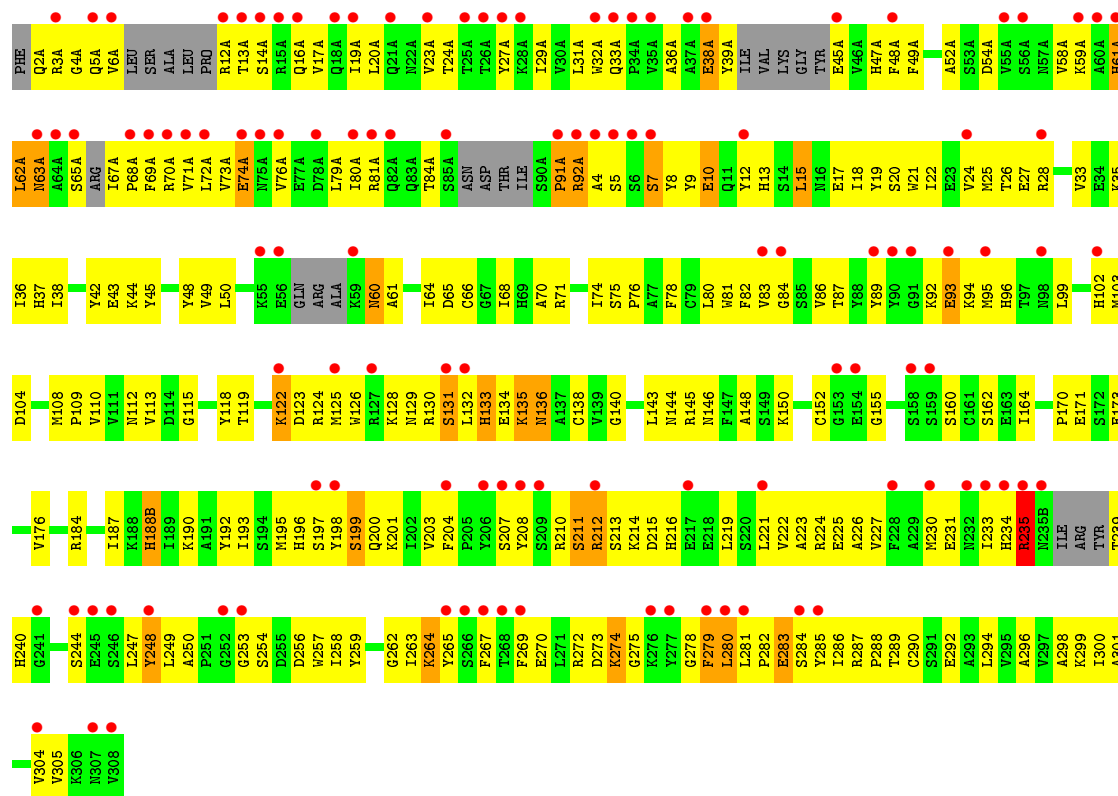


#### • Molecule 1: Carboxypeptidase B2



#### • Molecule 1: Carboxypeptidase B2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.47Å 146.47Å 231.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.86 – 2.50 19.86 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.86-2.50) 99.7 (19.86-2.50)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.50Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.205 , 0.243 0.208 , 0.244	Depositor DCC
$R_{free}$ test set	4345 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.6	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 83.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11015	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: ZN, BMA, NAG, MLI, NDG, SO4, FUL

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	0.37	0/3367	0.51	0/4560
1	B	0.34	0/3364	0.49	0/4557
1	C	0.24	0/3147	0.43	0/4261
All	All	0.32	0/9878	0.48	0/13378

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	92(A)	ARG	Peptide

### 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	A	3278	0	3194	99	0
1	B	3275	0	3183	96	0
1	C	3068	0	2926	218	0
2	A	28	0	25	0	0
2	B	28	0	25	1	0
3	A	24	0	22	1	0
4	A	28	0	25	2	0
4	B	28	0	25	2	0
5	A	38	0	34	0	0
6	B	39	0	34	2	0
7	B	14	0	13	2	0
8	C	14	0	13	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
10	A	45	0	0	2	0
10	B	55	0	0	0	0
10	C	10	0	0	1	0
11	A	7	0	2	0	0
11	B	7	0	2	1	0
11	C	7	0	2	0	0
12	A	484	0	0	19	0
12	B	417	0	0	19	0
12	C	118	0	0	17	0
All	All	11015	0	9525	415	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 21.

The worst 5 of 415 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)
1:A:75(A):ASN:ND2	1:A:78(A):ASP:H	1.55	1.03
1:C:281:LEU:HD12	1:C:282:PRO:HD2	1.54	0.89
1:C:201:LYS:H	1:C:270:GLU:HB2	1.39	0.87
1:C:136:ASN:HB2	1:C:160:SER:OG	1.77	0.84
1:C:75:SER:HB3	1:C:76:PRO:HD3	1.60	0.83

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	399/401 (100%)	386 (97%)	12 (3%)	1 (0%)	46	68
1	B	399/401 (100%)	373 (94%)	20 (5%)	6 (2%)	13	22
1	C	365/401 (91%)	304 (83%)	47 (13%)	14 (4%)	4	5
All	All	1163/1203 (97%)	1063 (91%)	79 (7%)	21 (2%)	11	18

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	SER
1	B	91(A)	PRO
1	B	199	SER
1	C	91(A)	PRO
1	C	131	SER

### 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	358/358 (100%)	328 (92%)	30 (8%)	14	25
1	B	357/358 (100%)	340 (95%)	17 (5%)	31	55
1	C	332/358 (93%)	310 (93%)	22 (7%)	21	38
All	All	1047/1074 (98%)	978 (93%)	69 (7%)	21	38

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	63(A)	ASN
1	B	57	GLN
1	C	235	ARG
1	B	92(A)	ARG
1	B	28	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	13	HIS
1	C	5(A)	GLN
1	C	216	HIS
1	B	188(B)	HIS
1	C	16(A)	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 ⓘ

16 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	$\# Z  > 2$
2	NAG	A	309	1,2	14,14,15	0.83	1 (7%)	15,19,21	1.31	3 (20%)
2	NDG	A	310	2	14,14,15	0.74	1 (7%)	15,19,21	0.73	1 (6%)
3	NAG	A	311	1,3	14,14,15	0.84	1 (7%)	15,19,21	0.75	0
3	FUL	A	312	3	10,10,11	0.54	0	13,14,16	0.44	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	313	1,4	14,14,15	0.57	0	15,19,21	0.85	1 (6%)
4	NAG	A	314	4	14,14,15	0.66	0	15,19,21	0.58	0
5	NDG	A	315	1,5	14,14,15	0.57	0	15,19,21	0.93	1 (6%)
5	NAG	A	316	5	14,14,15	0.57	0	15,19,21	0.72	1 (6%)
5	FUL	A	317	5	10,10,11	0.62	0	13,14,16	0.63	0
6	NAG	B	309	1,6	14,14,15	0.53	0	15,19,21	0.86	1 (6%)
6	NAG	B	310	6	14,14,15	0.71	0	15,19,21	1.01	0
6	BMA	B	311	6	11,11,12	0.78	0	15,15,17	1.04	2 (13%)
2	NAG	B	312	1,2	14,14,15	0.77	0	15,19,21	1.32	2 (13%)
2	NDG	B	313	2	14,14,15	0.72	0	15,19,21	0.89	1 (6%)
4	NAG	B	314	1,4	14,14,15	0.63	0	15,19,21	0.72	1 (6%)
4	NAG	B	315	4	14,14,15	0.65	0	15,19,21	0.63	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
2	NAG	A	309	1,2	-	0/6/23/26	0/1/1/1
2	NDG	A	310	2	-	0/6/23/26	0/1/1/1
3	NAG	A	311	1,3	-	0/6/23/26	0/1/1/1
3	FUL	A	312	3	-	0/0/17/20	0/1/1/1
4	NAG	A	313	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	314	4	-	0/6/23/26	0/1/1/1
5	NDG	A	315	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	316	5	-	0/6/23/26	0/1/1/1
5	FUL	A	317	5	-	0/0/17/20	0/1/1/1
6	NAG	B	309	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	310	6	-	0/6/23/26	0/1/1/1
6	BMA	B	311	6	-	0/2/19/22	0/1/1/1
2	NAG	B	312	1,2	-	0/6/23/26	0/1/1/1
2	NDG	B	313	2	-	0/6/23/26	0/1/1/1
4	NAG	B	314	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	315	4	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	310	NDG	C1-C2	2.02	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	309	NAG	C1-C2	2.23	1.55	1.52
3	A	311	NAG	C1-C2	2.42	1.55	1.52

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	313	NDG	C2-N2-C7	-2.53	119.82	123.11
5	A	315	NDG	C2-N2-C7	-2.52	119.83	123.11
6	B	309	NAG	C2-N2-C7	-2.46	119.90	123.11
2	A	309	NAG	C4-C3-C2	-2.38	107.65	111.34
5	A	316	NAG	C2-N2-C7	-2.29	120.12	123.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	311	NAG	1	0
4	A	313	NAG	2	0
4	A	314	NAG	2	0
6	B	309	NAG	1	0
6	B	310	NAG	2	0
6	B	311	BMA	1	0
2	B	312	NAG	1	0
4	B	314	NAG	2	0

## 5.6 Ligand geometry

Of 30 ligands modelled in this entry, 3 are monoatomic - leaving 27 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
10	SO4	A	319	-	4,4,4	0.17	0	6,6,6	0.13	0
10	SO4	A	320	-	4,4,4	0.27	0	6,6,6	0.20	0
10	SO4	A	321	-	4,4,4	0.20	0	6,6,6	0.08	0
10	SO4	A	322	-	4,4,4	0.29	0	6,6,6	0.14	0
10	SO4	A	323	-	4,4,4	0.17	0	6,6,6	0.18	0
10	SO4	A	324	-	4,4,4	0.18	0	6,6,6	0.09	0
10	SO4	A	325	-	4,4,4	0.16	0	6,6,6	0.06	0
10	SO4	A	326	-	4,4,4	0.19	0	6,6,6	0.09	0
10	SO4	A	327	-	4,4,4	0.21	0	6,6,6	0.17	0
11	MLI	A	328	9	0,6,6	0.00	-	0,7,7	0.00	-
7	NAG	B	316	1	14,14,15	0.55	0	15,19,21	0.79	0
10	SO4	B	318	-	4,4,4	0.15	0	6,6,6	0.18	0
10	SO4	B	319	-	4,4,4	0.14	0	6,6,6	0.15	0
10	SO4	B	320	-	4,4,4	0.22	0	6,6,6	0.19	0
10	SO4	B	321	-	4,4,4	0.20	0	6,6,6	0.10	0
10	SO4	B	322	-	4,4,4	0.23	0	6,6,6	0.06	0
10	SO4	B	323	-	4,4,4	0.21	0	6,6,6	0.10	0
10	SO4	B	324	-	4,4,4	0.23	0	6,6,6	0.12	0
10	SO4	B	325	-	4,4,4	0.21	0	6,6,6	0.10	0
10	SO4	B	326	-	4,4,4	0.19	0	6,6,6	0.09	0
10	SO4	B	327	-	4,4,4	0.18	0	6,6,6	0.13	0
10	SO4	B	328	-	4,4,4	0.19	0	6,6,6	0.09	0
11	MLI	B	329	-	0,6,6	0.00	-	0,7,7	0.00	-
8	NDG	C	309	1	14,14,15	0.48	0	15,19,21	0.75	1 (6%)
10	SO4	C	311	-	4,4,4	0.20	0	6,6,6	0.08	0
10	SO4	C	312	-	4,4,4	0.23	0	6,6,6	0.13	0
11	MLI	C	313	-	0,6,6	0.00	-	0,7,7	0.00	-

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
10	SO4	A	319	-	-	0/0/0/0	0/0/0/0
10	SO4	A	320	-	-	0/0/0/0	0/0/0/0
10	SO4	A	321	-	-	0/0/0/0	0/0/0/0
10	SO4	A	322	-	-	0/0/0/0	0/0/0/0
10	SO4	A	323	-	-	0/0/0/0	0/0/0/0
10	SO4	A	324	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	SO4	A	325	-	-	0/0/0/0	0/0/0/0
10	SO4	A	326	-	-	0/0/0/0	0/0/0/0
10	SO4	A	327	-	-	0/0/0/0	0/0/0/0
11	MLI	A	328	9	-	0/0/4/4	0/0/0/0
7	NAG	B	316	1	-	0/6/23/26	0/1/1/1
10	SO4	B	318	-	-	0/0/0/0	0/0/0/0
10	SO4	B	319	-	-	0/0/0/0	0/0/0/0
10	SO4	B	320	-	-	0/0/0/0	0/0/0/0
10	SO4	B	321	-	-	0/0/0/0	0/0/0/0
10	SO4	B	322	-	-	0/0/0/0	0/0/0/0
10	SO4	B	323	-	-	0/0/0/0	0/0/0/0
10	SO4	B	324	-	-	0/0/0/0	0/0/0/0
10	SO4	B	325	-	-	0/0/0/0	0/0/0/0
10	SO4	B	326	-	-	0/0/0/0	0/0/0/0
10	SO4	B	327	-	-	0/0/0/0	0/0/0/0
10	SO4	B	328	-	-	0/0/0/0	0/0/0/0
11	MLI	B	329	-	-	0/0/4/4	0/0/0/0
8	NDG	C	309	1	-	1/6/23/26	0/1/1/1
10	SO4	C	311	-	-	0/0/0/0	0/0/0/0
10	SO4	C	312	-	-	0/0/0/0	0/0/0/0
11	MLI	C	313	-	-	0/0/4/4	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	309	NDG	C2-N2-C7	-2.44	119.93	123.11

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	309	NDG	O7-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	323	SO4	1	0
10	A	327	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	316	NAG	2	0
11	B	329	MLI	1	0
10	C	311	SO4	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	A	401/401 (100%)	-0.25	6 (1%) 76 79	29, 44, 66, 87	0
1	B	401/401 (100%)	-0.22	9 (2%) 65 69	30, 49, 70, 93	0
1	C	379/401 (94%)	1.47	114 (30%) 1 0	72, 123, 156, 160	0
All	All	1181/1203 (98%)	0.31	129 (10%) 7 7	29, 56, 150, 160	0

The worst 5 of 129 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	37(A)	ALA	8.8
1	C	19(A)	ILE	8.2
1	C	56(A)	SER	8.1
1	C	228	PHE	8.0
1	C	60(A)	ALA	7.9

### 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	B	314	14/15	0.77	0.40	3.24	97,99,101,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	313	14/15	0.76	0.31	2.04	95,97,99,101	0
3	NAG	A	311	14/15	0.76	0.45	-	88,92,94,98	0
3	FUL	A	312	10/11	0.74	0.61	-	100,101,102,102	0
5	NAG	A	316	14/15	0.75	0.74	-	102,103,104,105	0
2	NDG	A	310	14/15	0.86	0.45	-	82,84,85,86	0
2	NAG	B	312	14/15	0.72	0.40	-	84,86,89,93	0
4	NAG	B	315	14/15	0.59	0.58	-	106,107,108,108	0
6	BMA	B	311	11/12	0.36	0.63	-	102,103,104,104	0
6	NAG	B	309	14/15	0.92	0.20	-	72,74,79,85	0
4	NAG	A	314	14/15	0.62	0.53	-	103,104,105,105	0
6	NAG	B	310	14/15	0.79	0.54	-	90,94,95,99	0
5	FUL	A	317	10/11	0.74	0.47	-	100,101,101,102	0
2	NAG	A	309	14/15	0.89	0.28	-	69,71,75,79	0
5	NDG	A	315	14/15	0.82	0.35	-	90,93,99,99	0
2	NDG	B	313	14/15	0.67	0.64	-	96,98,99,99	0

## 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( $\text{\AA}^2$ )	Q<0.9
11	MLI	A	328	7/7	0.86	0.34	5.11	72,73,74,74	0
11	MLI	B	329	7/7	0.87	0.27	2.28	66,67,68,68	0
9	ZN	A	318	1/1	0.99	0.10	1.04	39,39,39,39	0
10	SO4	B	319	5/5	0.99	0.14	0.42	73,74,74,75	0
10	SO4	B	324	5/5	0.92	0.14	0.10	103,103,104,104	0
10	SO4	C	312	5/5	0.78	0.23	-0.21	136,136,136,136	0
10	SO4	B	325	5/5	0.98	0.15	-0.33	118,118,118,118	0
10	SO4	A	322	5/5	0.97	0.12	-0.41	86,86,86,87	0
11	MLI	C	313	7/7	0.94	0.21	-0.47	109,109,109,109	0
10	SO4	A	319	5/5	0.99	0.09	-0.76	51,52,52,53	0
10	SO4	A	320	5/5	0.97	0.08	-1.20	71,72,72,72	0
9	ZN	C	310	1/1	0.90	0.09	-1.42	110,110,110,110	0
10	SO4	B	318	5/5	0.99	0.07	-1.56	58,58,59,60	0
10	SO4	A	326	5/5	0.94	0.32	-	147,147,147,147	0
10	SO4	A	327	5/5	0.78	0.21	-	98,99,99,99	0
10	SO4	B	328	5/5	0.85	0.17	-	140,140,140,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
10	SO4	B	327	5/5	0.94	0.20	-	94,94,95,95	0
10	SO4	A	321	5/5	0.97	0.08	-	80,81,81,81	0
10	SO4	B	326	5/5	0.94	0.12	-	129,129,129,129	0
10	SO4	C	311	5/5	0.96	0.16	-	110,110,110,110	0
9	ZN	B	317	1/1	0.99	0.10	-	39,39,39,39	0
10	SO4	B	321	5/5	0.98	0.19	-	100,100,100,100	0
7	NAG	B	316	14/15	0.78	0.48	-	85,88,89,90	0
10	SO4	B	322	5/5	0.90	0.27	-	127,127,127,127	0
10	SO4	A	325	5/5	0.95	0.17	-	114,114,114,114	0
10	SO4	A	323	5/5	0.95	0.15	-	92,92,93,93	0
8	NDG	C	309	14/15	0.53	0.46	-	151,152,152,152	0
10	SO4	B	323	5/5	0.96	0.13	-	105,105,105,105	0
10	SO4	A	324	5/5	0.96	0.15	-	80,80,81,81	0
10	SO4	B	320	5/5	0.98	0.11	-	73,73,74,74	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.