



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 08:32 AM UTC

PDB ID : 3D67 / pdb\_00003d67  
Title : Crystal structure of Thrombin-Activatable Fibrinolysis Inhibitor (TAFI) in complex with 2-guanidino-ethyl-mercaptosuccinic acid (GEMSA)  
Authors : Brondijk, T.H.C.; Huizinga, E.G.  
Deposited on : 2008-05-19  
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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

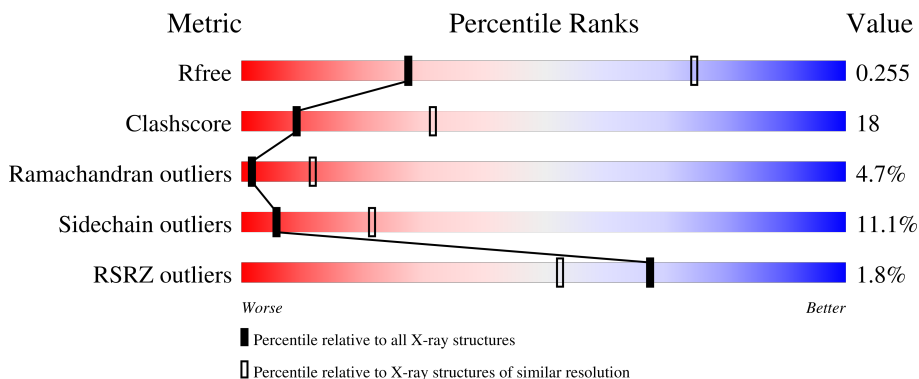
# 1 Overall quality at a glance

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))
$R_{free}$	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	424	
1	B	424	
1	C	424	

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
2	NAG	A	603	X	-	-	-
2	NAG	C	601	X	-	-	-

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 9940 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
			Total	C	N	O	S			
1	A	401	3246	2078	555	601	12	0	0	0
1	B	401	3246	2078	555	601	12	0	0	0
1	C	401	3246	2078	555	601	12	0	0	0

There are 75 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	GLY	-	expression tag	UNP Q96IY4
A	-21	SER	-	expression tag	UNP Q96IY4
A	-20	HIS	-	expression tag	UNP Q96IY4
A	-19	HIS	-	expression tag	UNP Q96IY4
A	-18	HIS	-	expression tag	UNP Q96IY4
A	-17	HIS	-	expression tag	UNP Q96IY4
A	-16	HIS	-	expression tag	UNP Q96IY4
A	-15	HIS	-	expression tag	UNP Q96IY4
A	-14	ASP	-	expression tag	UNP Q96IY4
A	-13	TYR	-	expression tag	UNP Q96IY4
A	-12	ASP	-	expression tag	UNP Q96IY4
A	-11	ILE	-	expression tag	UNP Q96IY4
A	-10	PRO	-	expression tag	UNP Q96IY4
A	-9	SER	-	expression tag	UNP Q96IY4
A	-8	SER	-	expression tag	UNP Q96IY4
A	-7	GLU	-	expression tag	UNP Q96IY4
A	-6	ASN	-	expression tag	UNP Q96IY4
A	-5	LEU	-	expression tag	UNP Q96IY4
A	-4	TYR	-	expression tag	UNP Q96IY4
A	-3	PHE	-	expression tag	UNP Q96IY4
A	-2	GLN	-	expression tag	UNP Q96IY4
A	-1	GLY	-	expression tag	UNP Q96IY4
A	0	SER	-	expression tag	UNP Q96IY4

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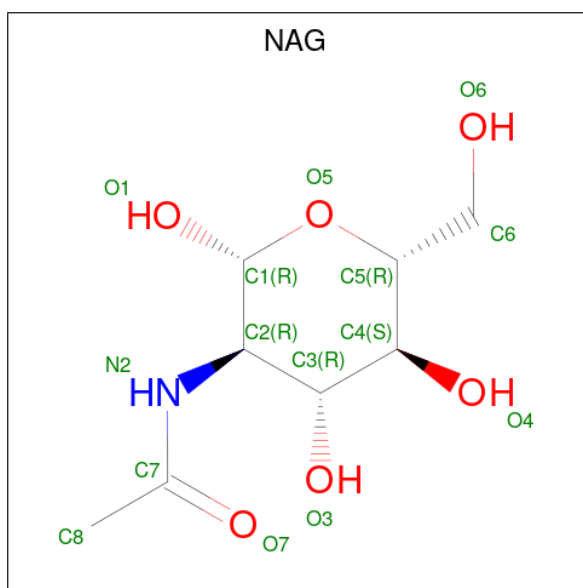
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	expression tag	UNP Q96IY4
A	147	THR	ALA	SEE REMARK 999	UNP Q96IY4
B	-22	GLY	-	expression tag	UNP Q96IY4
B	-21	SER	-	expression tag	UNP Q96IY4
B	-20	HIS	-	expression tag	UNP Q96IY4
B	-19	HIS	-	expression tag	UNP Q96IY4
B	-18	HIS	-	expression tag	UNP Q96IY4
B	-17	HIS	-	expression tag	UNP Q96IY4
B	-16	HIS	-	expression tag	UNP Q96IY4
B	-15	HIS	-	expression tag	UNP Q96IY4
B	-14	ASP	-	expression tag	UNP Q96IY4
B	-13	TYR	-	expression tag	UNP Q96IY4
B	-12	ASP	-	expression tag	UNP Q96IY4
B	-11	ILE	-	expression tag	UNP Q96IY4
B	-10	PRO	-	expression tag	UNP Q96IY4
B	-9	SER	-	expression tag	UNP Q96IY4
B	-8	SER	-	expression tag	UNP Q96IY4
B	-7	GLU	-	expression tag	UNP Q96IY4
B	-6	ASN	-	expression tag	UNP Q96IY4
B	-5	LEU	-	expression tag	UNP Q96IY4
B	-4	TYR	-	expression tag	UNP Q96IY4
B	-3	PHE	-	expression tag	UNP Q96IY4
B	-2	GLN	-	expression tag	UNP Q96IY4
B	-1	GLY	-	expression tag	UNP Q96IY4
B	0	SER	-	expression tag	UNP Q96IY4
B	1	ALA	-	expression tag	UNP Q96IY4
B	147	THR	ALA	SEE REMARK 999	UNP Q96IY4
C	-22	GLY	-	expression tag	UNP Q96IY4
C	-21	SER	-	expression tag	UNP Q96IY4
C	-20	HIS	-	expression tag	UNP Q96IY4
C	-19	HIS	-	expression tag	UNP Q96IY4
C	-18	HIS	-	expression tag	UNP Q96IY4
C	-17	HIS	-	expression tag	UNP Q96IY4
C	-16	HIS	-	expression tag	UNP Q96IY4
C	-15	HIS	-	expression tag	UNP Q96IY4
C	-14	ASP	-	expression tag	UNP Q96IY4
C	-13	TYR	-	expression tag	UNP Q96IY4
C	-12	ASP	-	expression tag	UNP Q96IY4
C	-11	ILE	-	expression tag	UNP Q96IY4
C	-10	PRO	-	expression tag	UNP Q96IY4
C	-9	SER	-	expression tag	UNP Q96IY4
C	-8	SER	-	expression tag	UNP Q96IY4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	GLU	-	expression tag	UNP Q96IY4
C	-6	ASN	-	expression tag	UNP Q96IY4
C	-5	LEU	-	expression tag	UNP Q96IY4
C	-4	TYR	-	expression tag	UNP Q96IY4
C	-3	PHE	-	expression tag	UNP Q96IY4
C	-2	GLN	-	expression tag	UNP Q96IY4
C	-1	GLY	-	expression tag	UNP Q96IY4
C	0	SER	-	expression tag	UNP Q96IY4
C	1	ALA	-	expression tag	UNP Q96IY4
C	147	THR	ALA	SEE REMARK 999	UNP Q96IY4

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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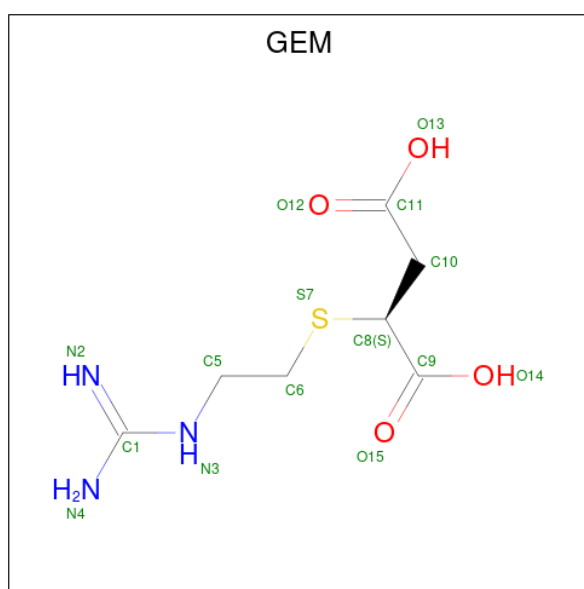
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

- Molecule 4 is (2-GUANIDINOETHYL)MERCAPTO)SUCCINIC ACID (CCD ID: GEM) (formula: C<sub>7</sub>H<sub>13</sub>N<sub>3</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	7	3	4	1		

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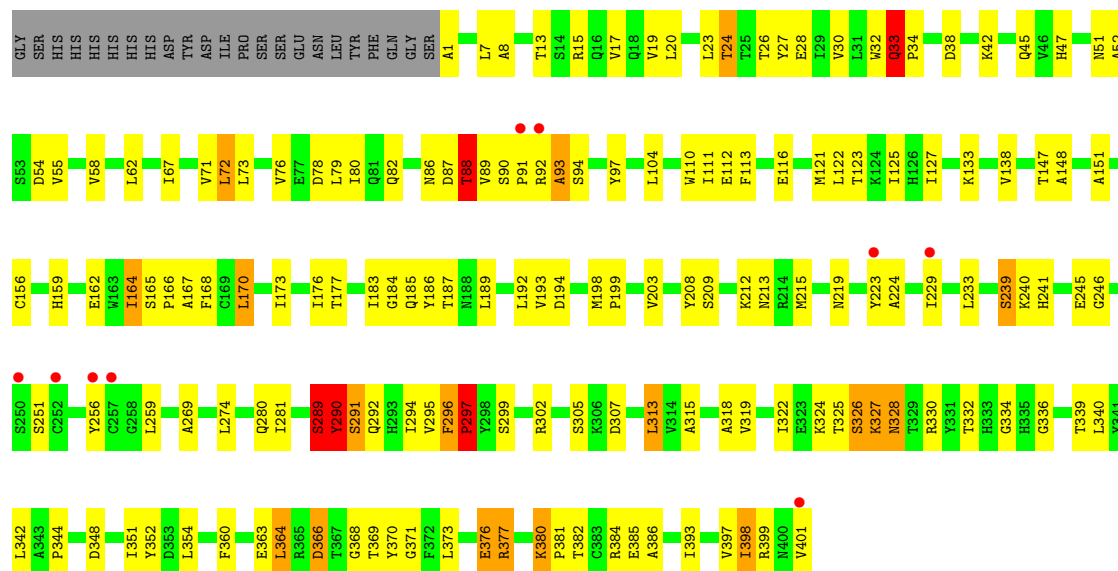
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	B	1	Total	C	N	O	S	0	0
			15	7	3	4	1		
4	C	1	Total	C	N	O	S	0	0
			15	7	3	4	1		





● Molecule 1: Carboxypeptidase B2



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.05Å 161.05Å 138.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.09 – 3.40 44.09 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.09-3.40) 99.5 (44.09-3.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 3.40Å)	Xtrriage
Refinement program	REFMAC 5.3.0008	Depositor
R, $R_{free}$	0.198 , 0.252 (Not available) , 0.255	Depositor DCC
$R_{free}$ test set	1472 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	112.6	Xtrriage
Anisotropy	0.317	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 155.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.047 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9940	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	118.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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, NAG, GEM

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	0.82	1/3334 (0.0%)	1.01	9/4530 (0.2%)
1	B	0.82	2/3334 (0.1%)	0.99	7/4530 (0.2%)
1	C	0.79	1/3334 (0.0%)	0.97	7/4530 (0.2%)
All	All	0.81	4/10002 (0.0%)	0.99	23/13590 (0.2%)

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	A	0	3
1	B	0	2
1	C	0	4
All	All	0	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	377	ARG	CZ-NH1	9.21	1.45	1.32
1	A	377	ARG	NE-CZ	5.76	1.39	1.33
1	B	270	VAL	CA-CB	5.74	1.61	1.54
1	C	398	ILE	CA-CB	-5.08	1.48	1.54

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	PHE	CA-C-N	8.48	130.44	119.84
1	A	296	PHE	C-N-CA	8.48	130.44	119.84
1	B	289	SER	N-CA-C	7.79	118.26	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	SER	N-CA-C	7.23	118.05	108.07
1	B	290	TYR	N-CA-C	6.68	125.03	110.80

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	289	SER	Peptide
1	A	326	SER	Peptide
1	A	33	GLN	Peptide
1	B	289	SER	Peptide
1	B	33	GLN	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	3246	0	3155	128	0
1	B	3246	0	3155	109	0
1	C	3246	0	3156	121	0
2	A	56	0	52	2	0
2	B	56	0	52	2	0
2	C	42	0	39	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	15	0	10	1	0
4	B	15	0	10	1	0
4	C	15	0	10	1	0
All	All	9940	0	9639	358	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 18.

The worst 5 of 358 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:C:121:MET:HE1	1:C:177:THR:HA	1.34	1.08
1:B:32:TRP:HE1	1:B:215:MET:HE2	1.22	1.05
1:C:121:MET:HE2	1:C:177:THR:HG22	1.40	1.03
1:A:198:MET:HE2	1:A:201:VAL:HA	1.47	0.94
1:C:121:MET:CE	1:C:177:THR:HG22	1.99	0.93

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	A	399/424 (94%)	337 (84%)	45 (11%)	17 (4%)	2	13
1	B	399/424 (94%)	338 (85%)	42 (10%)	19 (5%)	2	11
1	C	399/424 (94%)	337 (84%)	42 (10%)	20 (5%)	1	10
All	All	1197/1272 (94%)	1012 (84%)	129 (11%)	56 (5%)	2	12

5 of 56 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	PRO
1	A	219	ASN
1	A	224	ALA
1	A	243	CYS
1	A	291	SER

### 5.3.2 Protein sidechains [i](#)

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	354/375 (94%)	315 (89%)	39 (11%)	6	22
1	B	354/375 (94%)	311 (88%)	43 (12%)	5	19
1	C	354/375 (94%)	318 (90%)	36 (10%)	7	25
All	All	1062/1125 (94%)	944 (89%)	118 (11%)	6	21

5 of 118 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	176	ILE
1	C	327	LYS
1	B	329	THR
1	C	326	SER
1	C	193	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	150	ASN
1	C	33	GLN
1	B	279	ASN
1	C	100	GLN
1	A	227	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 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
2	NAG	B	602	1	14,14,15	1.01	1 (7%)	17,19,21	1.27	2 (11%)
2	NAG	A	604	1	14,14,15	0.58	0	17,19,21	1.57	2 (11%)
2	NAG	B	604	1	14,14,15	0.64	0	17,19,21	1.40	2 (11%)
2	NAG	C	601	1	14,14,15	0.60	0	17,19,21	1.30	1 (5%)
4	GEM	A	660	3	14,14,14	0.87	1 (7%)	11,17,17	1.02	1 (9%)
2	NAG	A	601	1	14,14,15	0.79	0	17,19,21	1.01	1 (5%)
2	NAG	A	603	1	14,14,15	1.04	1 (7%)	17,19,21	1.51	3 (17%)
4	GEM	C	660	3	14,14,14	0.90	1 (7%)	11,17,17	0.96	0
2	NAG	C	604	1	14,14,15	0.56	0	17,19,21	1.37	2 (11%)
2	NAG	C	602	1	14,14,15	0.93	1 (7%)	17,19,21	1.70	4 (23%)
4	GEM	B	660	3	14,14,14	0.92	0	11,17,17	1.11	1 (9%)
2	NAG	B	603	1	14,14,15	0.48	0	17,19,21	1.36	4 (23%)
2	NAG	B	601	1	14,14,15	0.82	0	17,19,21	1.80	3 (17%)
2	NAG	A	602	1	14,14,15	0.60	0	17,19,21	1.41	2 (11%)

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	B	602	1	-	3/6/23/26	0/1/1/1
2	NAG	A	604	1	-	3/6/23/26	0/1/1/1
2	NAG	B	604	1	-	4/6/23/26	0/1/1/1
2	NAG	C	601	1	1/1/5/7	2/6/23/26	0/1/1/1
4	GEM	A	660	3	-	12/15/15/15	-
2	NAG	A	603	1	1/1/5/7	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	601	1	-	2/6/23/26	0/1/1/1
4	GEM	C	660	3	-	7/15/15/15	-
2	NAG	C	604	1	-	2/6/23/26	0/1/1/1
2	NAG	C	602	1	-	4/6/23/26	0/1/1/1
4	GEM	B	660	3	-	10/15/15/15	-
2	NAG	B	603	1	-	3/6/23/26	0/1/1/1
2	NAG	B	601	1	-	4/6/23/26	0/1/1/1
2	NAG	A	602	1	-	1/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	603	NAG	C1-C2	2.95	1.56	1.52
2	B	602	NAG	C1-C2	2.62	1.55	1.52
2	C	602	NAG	C1-C2	2.36	1.55	1.52
4	A	660	GEM	O13-C11	-2.14	1.23	1.30
4	C	660	GEM	O13-C11	-2.03	1.24	1.30

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	NAG	C1-O5-C5	5.55	119.63	112.19
2	A	604	NAG	C1-O5-C5	5.11	119.03	112.19
2	A	602	NAG	C1-O5-C5	4.79	118.60	112.19
2	C	602	NAG	C2-N2-C7	4.46	128.88	122.90
2	C	601	NAG	C1-O5-C5	4.37	118.05	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	603	NAG	C1
2	C	601	NAG	C1

5 of 60 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	NAG	C8-C7-N2-C2
2	A	601	NAG	O7-C7-N2-C2
2	A	603	NAG	C3-C2-N2-C7
2	A	604	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	A	604	NAG	O7-C7-N2-C2

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	602	NAG	2	0
2	A	604	NAG	2	0
2	C	601	NAG	1	0
4	A	660	GEM	1	0
4	C	660	GEM	1	0
2	C	604	NAG	1	0
2	C	602	NAG	3	0
4	B	660	GEM	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	401/424 (94%)	-0.06	6 (1%) 72 57	94, 116, 129, 138	0
1	B	401/424 (94%)	-0.03	7 (1%) 69 54	97, 115, 142, 153	0
1	C	401/424 (94%)	-0.08	9 (2%) 62 47	90, 119, 139, 148	0
All	All	1203/1272 (94%)	-0.06	22 (1%) 67 53	90, 117, 137, 153	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	257	CYS	4.3
1	B	341	TYR	3.7
1	A	300	TYR	3.5
1	C	401	VAL	3.2
1	B	95	ALA	3.0

### 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 oligosaccharides 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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	A	603	14/15	0.47	0.10	116,121,122,122	0
2	NAG	A	602	14/15	0.63	0.10	127,129,131,131	0
2	NAG	A	601	14/15	0.69	0.08	129,130,131,131	0
2	NAG	C	604	14/15	0.72	0.12	87,91,92,93	0
2	NAG	B	603	14/15	0.73	0.09	122,122,123,124	0
2	NAG	B	604	14/15	0.74	0.11	111,112,114,114	0
2	NAG	C	601	14/15	0.76	0.08	133,134,134,134	0
2	NAG	B	602	14/15	0.76	0.09	122,123,126,127	0
2	NAG	A	604	14/15	0.81	0.12	97,99,100,101	0
2	NAG	C	602	14/15	0.83	0.09	133,135,136,136	0
2	NAG	B	601	14/15	0.87	0.09	106,110,112,113	0
4	GEM	C	660	15/15	0.92	0.17	116,122,124,125	0
4	GEM	A	660	15/15	0.93	0.16	102,107,112,112	0
4	GEM	B	660	15/15	0.94	0.17	121,124,126,126	0
3	ZN	C	501	1/1	0.98	0.04	126,126,126,126	0
3	ZN	B	501	1/1	0.98	0.04	120,120,120,120	0
3	ZN	A	501	1/1	0.99	0.04	117,117,117,117	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.