



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 21, 2016 – 04:40 PM EDT

PDB ID : 5EDM  
Title : Crystal structure of prothrombin deletion mutant residues 154-167 ( Form I )  
Authors : Pozzi, N.; Chen, Z.; Di Cera, E.  
Deposited on : 2015-10-21  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0122  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

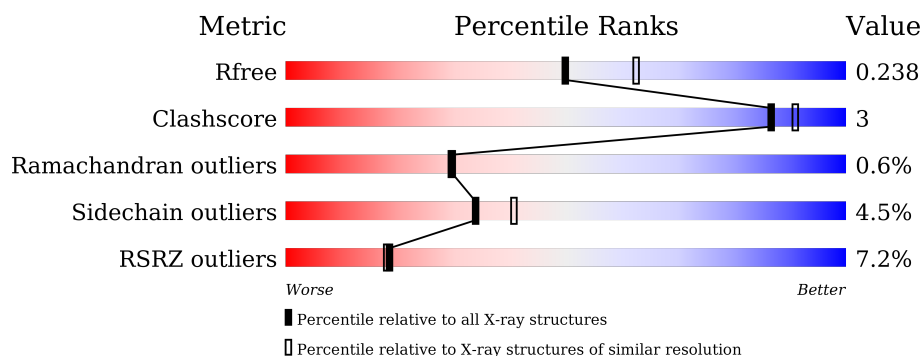
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	568	

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
4	SO4	A	615	-	-	-	X
4	SO4	A	616	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	617	-	-	-	X
5	GOL	A	620	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5005 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 Prothrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	0	0	0
			4414	2755	766	860	33			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	122	MET	THR	conflict	UNP P00734
A	?	-	PRO	deletion	UNP P00734
A	?	-	ARG	deletion	UNP P00734
A	?	-	SER	deletion	UNP P00734
A	?	-	GLU	deletion	UNP P00734
A	?	-	GLY	deletion	UNP P00734
A	?	-	SER	deletion	UNP P00734
A	?	-	SER	deletion	UNP P00734
A	?	-	VAL	deletion	UNP P00734
A	?	-	ASN	deletion	UNP P00734
A	?	-	LEU	deletion	UNP P00734
A	?	-	SER	deletion	UNP P00734
A	?	-	PRO	deletion	UNP P00734
A	?	-	PRO	deletion	UNP P00734
A	?	-	LEU	deletion	UNP P00734
A	566	TYR	-	expression tag	UNP P00734
A	567	LEU	-	expression tag	UNP P00734
A	568	GLU	-	expression tag	UNP P00734

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

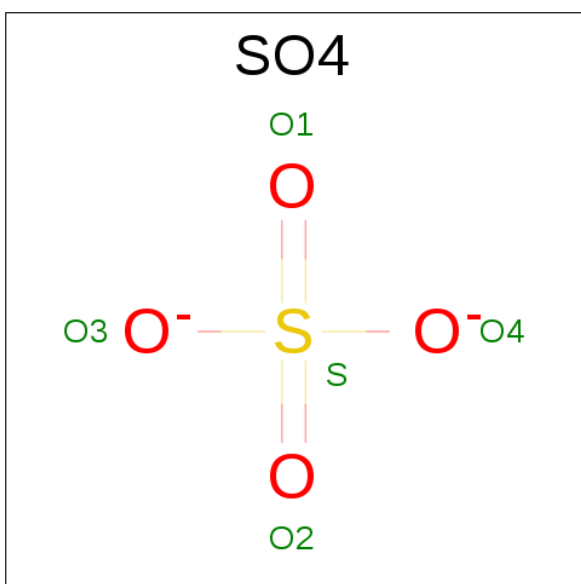
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	Mg	0	0
			6	6		

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



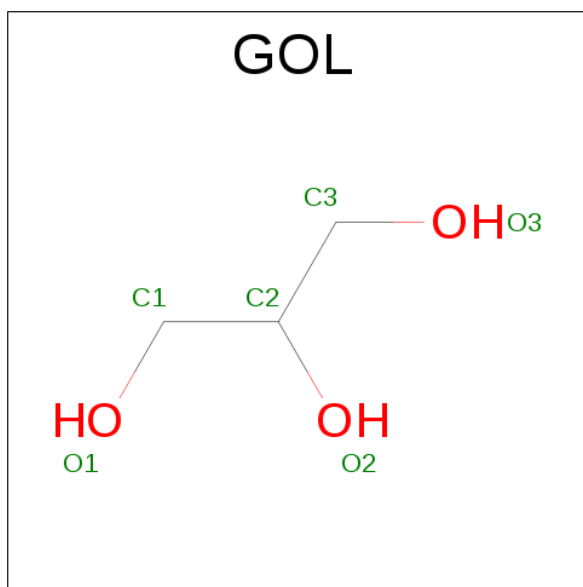
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

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



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0

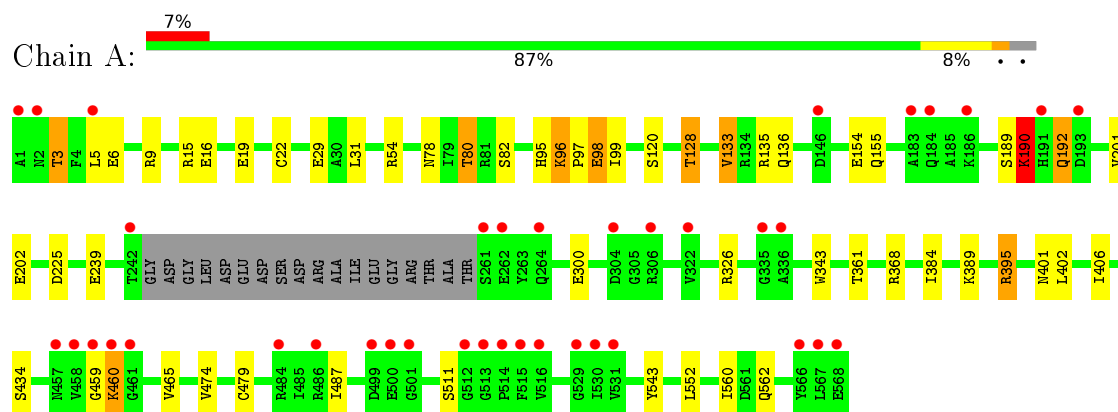
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	464	Total 464	O 464	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: Prothrombin





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.88Å 168.69Å 144.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.07 – 2.20 28.72 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (92.07-2.20) 98.0 (28.72-2.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.196 , 0.236 0.205 , 0.238	Depositor DCC
$R_{free}$ test set	3409 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.9	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 66772 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5005	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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: GOL, MG, CGU, NAG, SO4

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	0.81	19/4393 (0.4%)	0.79	3/5941 (0.1%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	99	ILE	C-O	-11.95	1.00	1.23
1	A	98	GLU	C-O	-11.60	1.01	1.23
1	A	98	GLU	CA-CB	-10.78	1.30	1.53
1	A	98	GLU	CB-CG	-10.70	1.31	1.52
1	A	96	LYS	C-O	-9.88	1.04	1.23
1	A	97	PRO	C-O	-9.72	1.03	1.23
1	A	98	GLU	CD-OE2	-8.70	1.16	1.25
1	A	98	GLU	CG-CD	-8.52	1.39	1.51
1	A	98	GLU	CD-OE1	-8.31	1.16	1.25
1	A	97	PRO	CA-CB	-8.15	1.37	1.53
1	A	97	PRO	CA-C	-7.81	1.37	1.52
1	A	97	PRO	CG-CD	-6.08	1.30	1.50
1	A	98	GLU	N-CA	-5.90	1.34	1.46
1	A	96	LYS	N-CA	-5.74	1.34	1.46
1	A	96	LYS	CA-CB	-5.57	1.41	1.53
1	A	95	HIS	C-N	-5.51	1.21	1.34
1	A	99	ILE	N-CA	-5.43	1.35	1.46
1	A	99	ILE	CA-C	-5.26	1.39	1.52
1	A	99	ILE	CB-CG1	-5.20	1.39	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	ASN	CB-CA-C	-7.58	95.24	110.40
1	A	97	PRO	CA-N-CD	-5.57	103.70	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	ARG	NE-CZ-NH1	5.15	122.87	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	4414	0	4151	24	0
2	A	6	0	0	0	0
3	A	70	0	63	0	0
4	A	45	0	0	0	0
5	A	6	0	8	0	0
6	A	464	0	0	3	0
All	All	5005	0	4222	24	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 3.

All (24) 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:29:CGU:HG	6:A:775:HOH:O	2.04	0.58
1:A:225:ASP:OD1	1:A:562:GLN:NE2	2.38	0.56
1:A:80:THR:HG23	1:A:136:GLN:OE1	2.07	0.55
1:A:80:THR:CG2	1:A:136:GLN:OE1	2.56	0.53
1:A:3:THR:HG23	1:A:6:CGU:CD1	2.42	0.50
1:A:82:SER:O	1:A:155:GLN:HA	2.12	0.49
1:A:459:GLY:O	1:A:460:LYS:C	2.51	0.48
1:A:474:VAL:HG21	1:A:543:TYR:CD1	2.48	0.48
1:A:128:THR:HG21	1:A:133:VAL:HG22	1.96	0.48
1:A:201:VAL:HG12	1:A:202:GLU:HG3	1.97	0.46
1:A:9:ARG:HD3	1:A:31:LEU:HA	1.97	0.46
1:A:16:CGU:O	1:A:22:CYS:HB3	2.17	0.45
1:A:190:LYS:HD3	1:A:190:LYS:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:GLU:OE2	6:A:702:HOH:O	2.20	0.44
1:A:343:TRP:CZ2	1:A:560:ILE:HG22	2.53	0.43
1:A:189:SER:HA	1:A:192:GLN:HG2	2.00	0.43
1:A:3:THR:HG23	1:A:6:CGU:CG	2.48	0.42
1:A:3:THR:CG2	1:A:6:CGU:CD1	2.97	0.42
1:A:368:ARG:HG2	1:A:384:ILE:HD12	2.02	0.42
1:A:15:ARG:NH1	1:A:19:CGU:OE11	2.53	0.42
1:A:487:ILE:HA	6:A:812:HOH:O	2.19	0.42
1:A:406:ILE:HD13	1:A:552:LEU:HD21	2.01	0.41
1:A:401:ASN:O	1:A:402:LEU:C	2.59	0.40
1:A:192:GLN:OE1	1:A:192:GLN:CA	2.70	0.40

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	536/568 (94%)	509 (95%)	24 (4%)	3 (1%)	30	29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	LYS
1	A	460	LYS
1	A	239	GLU

### 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	463/476 (97%)	442 (96%)	21 (4%)	34	41

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	5	LEU
1	A	54	ARG
1	A	80	THR
1	A	96	LYS
1	A	98	GLU
1	A	120	SER
1	A	128	THR
1	A	133	VAL
1	A	135	ARG
1	A	154	GLU
1	A	190	LYS
1	A	192	GLN
1	A	326	ARG
1	A	361	THR
1	A	389	LYS
1	A	395	ARG
1	A	434	SER
1	A	465	VAL
1	A	479	CYS
1	A	511	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	380	ASN
1	A	562	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

10 non-standard protein/DNA/RNA residues 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
1	CGU	A	14	1,2	3,11,12	0.45	0	4,14,16	1.26	1 (25%)
1	CGU	A	16	1,2	3,11,12	0.72	0	4,14,16	1.22	0
1	CGU	A	19	1,2	3,11,12	0.60	0	4,14,16	1.05	0
1	CGU	A	20	1,2	3,11,12	0.28	0	4,14,16	1.30	1 (25%)
1	CGU	A	25	1,2	3,11,12	0.54	0	4,14,16	1.37	1 (25%)
1	CGU	A	26	1,2	3,11,12	0.38	0	4,14,16	1.01	0
1	CGU	A	29	1,2	3,11,12	0.95	0	4,14,16	2.94	2 (50%)
1	CGU	A	32	1,2	3,11,12	0.69	0	4,14,16	1.22	0
1	CGU	A	6	1	3,11,12	0.62	0	4,14,16	1.37	1 (25%)
1	CGU	A	7	1	3,11,12	0.70	0	4,14,16	0.80	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
1	CGU	A	14	1,2	-	0/4/14/16	0/0/0/0
1	CGU	A	16	1,2	-	0/4/14/16	0/0/0/0
1	CGU	A	19	1,2	-	0/4/14/16	0/0/0/0
1	CGU	A	20	1,2	-	0/4/14/16	0/0/0/0
1	CGU	A	25	1,2	-	0/4/14/16	0/0/0/0
1	CGU	A	26	1,2	-	0/4/14/16	0/0/0/0
1	CGU	A	29	1,2	-	0/4/14/16	0/0/0/0
1	CGU	A	32	1,2	-	0/4/14/16	0/0/0/0
1	CGU	A	6	1	-	0/4/14/16	0/0/0/0
1	CGU	A	7	1	-	0/4/14/16	0/0/0/0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	CGU	CB-CG-CD2	-3.50	105.77	112.83
1	A	6	CGU	O-C-CA	-2.53	118.94	125.72
1	A	14	CGU	O-C-CA	-2.35	119.41	125.72
1	A	25	CGU	O-C-CA	-2.21	119.79	125.72
1	A	20	CGU	O-C-CA	-2.12	120.05	125.72
1	A	29	CGU	CB-CG-CD1	4.32	121.55	112.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	16	CGU	1	0
1	A	19	CGU	1	0
1	A	29	CGU	1	0
1	A	6	CGU	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 6 are monoatomic - leaving 15 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	$\# Z  > 2$
3	NAG	A	607	1	14,14,15	0.76	0	15,19,21	1.88	5 (33%)
3	NAG	A	608	1,3	14,14,15	0.98	1 (7%)	15,19,21	1.29	2 (13%)
3	NAG	A	609	3	14,14,15	0.86	1 (7%)	15,19,21	1.37	1 (6%)
3	NAG	A	610	1,3	14,14,15	0.49	0	15,19,21	0.95	0
3	NAG	A	611	3	14,14,15	0.51	0	15,19,21	0.84	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	A	612	-	4,4,4	0.46	0	6,6,6	0.27	0
4	SO4	A	613	-	4,4,4	0.46	0	6,6,6	0.76	0
4	SO4	A	614	-	4,4,4	0.44	0	6,6,6	0.43	0
4	SO4	A	615	-	4,4,4	0.45	0	6,6,6	0.27	0
4	SO4	A	616	-	4,4,4	0.71	0	6,6,6	3.48	4 (66%)
4	SO4	A	617	-	4,4,4	0.43	0	6,6,6	0.29	0
4	SO4	A	618	-	4,4,4	0.40	0	6,6,6	1.15	1 (16%)
4	SO4	A	619	-	4,4,4	0.50	0	6,6,6	0.67	0
5	GOL	A	620	-	5,5,5	0.42	0	5,5,5	0.23	0
4	SO4	A	621	-	4,4,4	0.59	0	6,6,6	0.21	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	A	607	1	-	0/6/23/26	0/1/1/1
3	NAG	A	608	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	609	3	-	0/6/23/26	0/1/1/1
3	NAG	A	610	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	611	3	-	0/6/23/26	0/1/1/1
4	SO4	A	612	-	-	0/0/0/0	0/0/0/0
4	SO4	A	613	-	-	0/0/0/0	0/0/0/0
4	SO4	A	614	-	-	0/0/0/0	0/0/0/0
4	SO4	A	615	-	-	0/0/0/0	0/0/0/0
4	SO4	A	616	-	-	0/0/0/0	0/0/0/0
4	SO4	A	617	-	-	0/0/0/0	0/0/0/0
4	SO4	A	618	-	-	0/0/0/0	0/0/0/0
4	SO4	A	619	-	-	0/0/0/0	0/0/0/0
5	GOL	A	620	-	-	0/4/4/4	0/0/0/0
4	SO4	A	621	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	609	NAG	C8-C7	2.82	1.56	1.50
3	A	608	NAG	C8-C7	3.07	1.57	1.50

All (14) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	616	SO4	O2-S-O1	-6.82	86.79	109.59
3	A	607	NAG	O5-C5-C4	-3.96	103.58	110.13
3	A	608	NAG	O5-C5-C4	-2.86	105.39	110.13
4	A	616	SO4	O4-S-O2	-2.85	85.46	110.02
4	A	616	SO4	O3-S-O2	-2.70	86.71	110.02
3	A	607	NAG	C3-C4-C5	-2.48	105.80	110.23
3	A	607	NAG	O4-C4-C5	2.07	114.68	109.23
3	A	611	NAG	C3-C4-C5	2.11	113.98	110.23
3	A	607	NAG	C6-C5-C4	2.19	118.48	112.99
4	A	618	SO4	O2-S-O1	2.21	116.95	109.59
3	A	607	NAG	C1-O5-C5	2.21	115.39	112.14
3	A	608	NAG	C6-C5-C4	2.33	118.83	112.99
4	A	616	SO4	O4-S-O3	2.90	120.79	109.09
3	A	609	NAG	C1-O5-C5	3.38	117.11	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	540/568 (95%)	0.03	39 (7%) 18 18	33, 53, 99, 127	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	459	GLY	6.3
1	A	458	VAL	6.3
1	A	242	THR	5.3
1	A	261	SER	4.7
1	A	262	GLU	4.0
1	A	460	LYS	3.9
1	A	193	ASP	3.9
1	A	1	ALA	3.8
1	A	500	GLU	3.8
1	A	184	GLN	3.7
1	A	191	HIS	3.6
1	A	501	GLY	3.6
1	A	183	ALA	3.4
1	A	186	LYS	3.3
1	A	531	VAL	3.1
1	A	530	ILE	3.1
1	A	514	PRO	3.0
1	A	568	GLU	3.0
1	A	566	TYR	2.9
1	A	304	ASP	2.9
1	A	484	ARG	2.8
1	A	2	ASN	2.8
1	A	146	ASP	2.8
1	A	529	GLY	2.6
1	A	499	ASP	2.6
1	A	513	GLY	2.6
1	A	322	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	516	VAL	2.5
1	A	515	PHE	2.4
1	A	567	LEU	2.4
1	A	306	ARG	2.3
1	A	486	ARG	2.3
1	A	335	GLY	2.3
1	A	5	LEU	2.2
1	A	512	GLY	2.1
1	A	264	GLN	2.1
1	A	457	ASN	2.1
1	A	336	ALA	2.1
1	A	461	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CGU	A	20	12/13	0.97	0.07	-	49,57,66,72	0
1	CGU	A	16	12/13	0.94	0.11	-	51,55,58,62	0
1	CGU	A	29	12/13	0.95	0.08	-	60,72,78,79	0
1	CGU	A	32	12/13	0.94	0.08	-	65,73,75,75	0
1	CGU	A	14	12/13	0.96	0.08	-	51,58,68,71	0
1	CGU	A	26	12/13	0.95	0.08	-	51,53,56,68	0
1	CGU	A	25	12/13	0.96	0.13	-	53,72,81,84	0
1	CGU	A	6	12/13	0.91	0.19	-	78,89,92,93	0
1	CGU	A	19	12/13	0.96	0.07	-	53,59,65,68	0
1	CGU	A	7	12/13	0.87	0.15	-	70,78,82,84	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	SO4	A	617	5/5	0.81	0.49	14.91	116,128,134,135	0
4	SO4	A	615	5/5	0.93	0.26	8.85	92,106,108,111	0
5	GOL	A	620	6/6	0.85	0.18	2.07	71,80,84,89	0
4	SO4	A	619	5/5	0.90	0.20	1.65	89,90,106,106	0
4	SO4	A	614	5/5	0.93	0.25	0.57	100,104,109,113	0
4	SO4	A	618	5/5	0.99	0.04	-1.37	60,62,68,68	0
2	MG	A	602	1/1	0.99	0.08	-	59,59,59,59	0
2	MG	A	603	1/1	0.67	0.35	-	75,75,75,75	0
3	NAG	A	608	14/15	0.82	0.19	-	73,87,93,113	0
3	NAG	A	611	14/15	0.81	0.47	-	118,136,139,141	0
4	SO4	A	621	5/5	0.91	0.10	-	69,73,85,98	0
3	NAG	A	607	14/15	0.58	0.32	-	66,79,90,99	0
2	MG	A	604	1/1	0.96	0.04	-	44,44,44,44	0
2	MG	A	605	1/1	0.95	0.11	-	61,61,61,61	0
4	SO4	A	616	5/5	0.78	0.49	-	147,158,159,159	0
3	NAG	A	609	14/15	0.74	0.47	-	111,126,136,139	0
3	NAG	A	610	14/15	0.93	0.19	-	70,79,96,118	0
2	MG	A	601	1/1	0.97	0.04	-	54,54,54,54	0
4	SO4	A	612	5/5	0.87	0.26	-	97,115,118,121	0
2	MG	A	606	1/1	0.89	0.03	-	50,50,50,50	0
4	SO4	A	613	5/5	0.97	0.12	-	57,71,81,93	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.