



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 09:35 AM BST

PDB ID : 4O03  
Title : Crystal structure of Ca<sup>2+</sup> bound prothrombin deletion mutant residues 146-167  
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Deposited on : 2013-12-13  
Resolution : 3.38 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

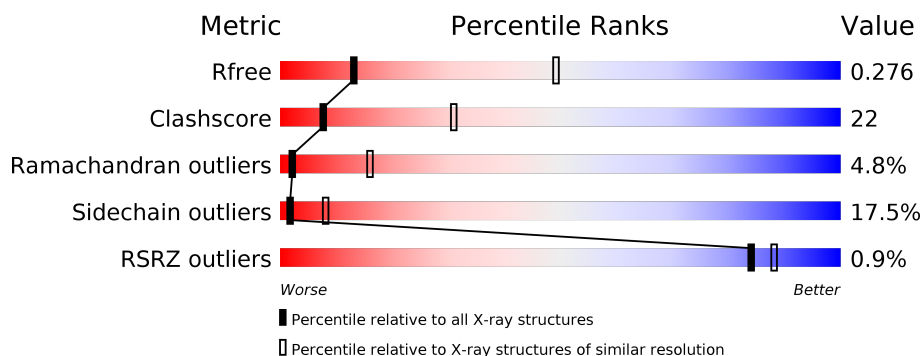
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.38 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))
$R_{free}$	130704	1691 (3.46-3.30)
Clashscore	141614	1762 (3.46-3.30)
Ramachandran outliers	138981	1732 (3.46-3.30)
Sidechain outliers	138945	1731 (3.46-3.30)
RSRZ outliers	127900	1635 (3.46-3.30)

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 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	557	<div> <div></div> <div>48%</div> <div>40%</div> <div>8%</div> <div>..</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4368 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.

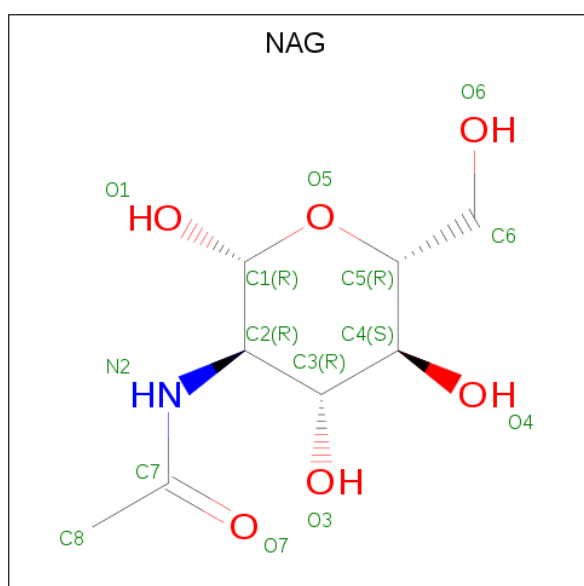
- Molecule 1 is a protein called Prothrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	539	Total	C	N	O	S	0	0	0
			4321	2696	751	843	31			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	Ca	0	0
			5	5		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (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		

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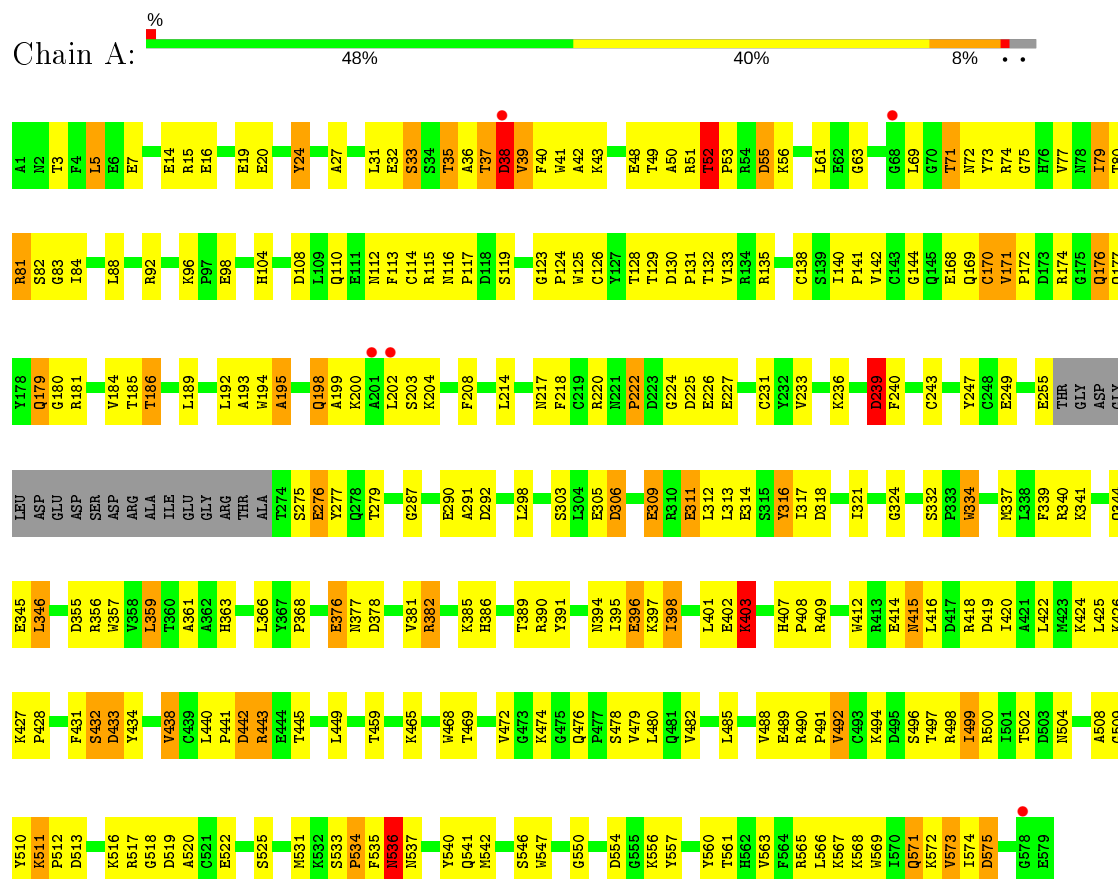
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	177.46 Å   89.43 Å   87.98 Å 90.00°   116.36°   90.00°	Depositor
Resolution (Å)	39.75 – 3.38 39.75 – 3.38	Depositor EDS
% Data completeness (in resolution range)	94.7 (39.75-3.38) 94.7 (39.75-3.38)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 3.40 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.233   ,   0.279 0.232   ,   0.276	Depositor DCC
$R_{free}$ test set	835 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	74.2	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 14.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	4368	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% 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: CA, CGU, NAG

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	0.69	0/4299	0.77	1/5813 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	170	CYS	CA-CB-SG	5.00	123.00	114.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	36	ALA	Peptide
1	A	52	THR	Peptide
1	A	69	LEU	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	4321	0	4057	185	0
2	A	5	0	0	0	0
3	A	42	0	39	0	0
All	All	4368	0	4096	185	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 22.

All (185) 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:382:ARG:HG2	1:A:382:ARG:HH21	1.08	1.08
1:A:52:THR:HG22	1:A:56:LYS:HD2	1.37	1.07
1:A:84:ILE:HG21	1:A:128:THR:HG23	1.38	1.05
1:A:418:ARG:HD2	1:A:504:ASN:HD22	1.26	1.00
1:A:418:ARG:HD2	1:A:504:ASN:ND2	1.78	0.98
1:A:489:GLU:HB2	1:A:492:VAL:HG23	1.49	0.94
1:A:311:GLU:O	1:A:311:GLU:HG3	1.74	0.87
1:A:489:GLU:HB2	1:A:492:VAL:CG2	2.03	0.87
1:A:52:THR:CG2	1:A:56:LYS:HD2	2.03	0.87
1:A:568:LYS:HA	1:A:571:GLN:HB2	1.58	0.83
1:A:382:ARG:HG2	1:A:382:ARG:NH2	1.88	0.79
1:A:361:ALA:HB1	1:A:419:ASP:OD1	1.83	0.79
1:A:40:PHE:HA	1:A:43:LYS:HB2	1.64	0.78
1:A:390:ARG:HB3	1:A:390:ARG:HH11	1.47	0.77
1:A:128:THR:HG22	1:A:130:ASP:H	1.52	0.75
1:A:39:VAL:HA	1:A:42:ALA:HB3	1.68	0.75
1:A:169:GLN:O	1:A:170:CYS:HB3	1.88	0.74
1:A:305:GLU:HG3	1:A:309:GLU:HG2	1.68	0.74
1:A:74:ARG:HD2	1:A:108:ASP:HB2	1.71	0.72
1:A:37:THR:HG23	1:A:40:PHE:HB3	1.72	0.72
1:A:84:ILE:HG21	1:A:128:THR:CG2	2.18	0.71
1:A:550:GLY:HA2	1:A:556:LYS:HB2	1.71	0.71
1:A:569:TRP:O	1:A:573:VAL:HG23	1.91	0.70
1:A:198:GLN:HA	1:A:202:LEU:HB2	1.72	0.70
1:A:195:ALA:O	1:A:200:LYS:HG3	1.92	0.70
1:A:52:THR:HG23	1:A:53:PRO:HD3	1.72	0.69
1:A:176:GLN:HE22	1:A:224:GLY:HA2	1.55	0.69
1:A:337:MET:SD	1:A:385:LYS:HD3	2.32	0.69
1:A:546:SER:OG	1:A:547:TRP:N	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:THR:CG2	1:A:40:PHE:HB3	2.23	0.69
1:A:357:TRP:CZ3	1:A:424:LYS:HB2	2.29	0.68
1:A:489:GLU:CB	1:A:492:VAL:HG23	2.21	0.68
1:A:497:THR:OG1	1:A:499:ILE:HG23	1.93	0.67
1:A:176:GLN:NE2	1:A:224:GLY:HA2	2.09	0.67
1:A:35:THR:O	1:A:37:THR:HG22	1.93	0.67
1:A:513:ASP:HB2	1:A:516:LYS:HB3	1.77	0.67
1:A:48:GLU:HB3	1:A:181:ARG:HD2	1.77	0.65
1:A:499:ILE:HG13	1:A:500:ARG:N	2.11	0.65
1:A:390:ARG:HB3	1:A:390:ARG:NH1	2.10	0.65
1:A:255:GLU:OE2	1:A:443:ARG:HD2	1.97	0.65
1:A:337:MET:CE	1:A:346:LEU:HD13	2.27	0.64
1:A:298:LEU:HG	1:A:433:ASP:HB3	1.78	0.64
1:A:84:ILE:CG2	1:A:128:THR:HG23	2.23	0.64
1:A:508:ALA:HB3	1:A:560:TYR:HE2	1.64	0.63
1:A:287:GLY:HA3	1:A:355:ASP:OD1	1.99	0.62
1:A:73:TYR:CZ	1:A:75:GLY:HA3	2.34	0.62
1:A:24:TYR:O	1:A:27:ALA:HB3	2.00	0.62
1:A:5:LEU:O	1:A:7:CGU:N	2.33	0.62
1:A:492:VAL:O	1:A:496:SER:HB3	2.00	0.61
1:A:337:MET:HE3	1:A:346:LEU:HD13	1.81	0.61
1:A:14:CGU:OE21	1:A:19:CGU:OE11	2.20	0.59
1:A:489:GLU:HB3	1:A:491:PRO:HD2	1.85	0.59
1:A:427:LYS:HE3	1:A:428:PRO:O	2.02	0.59
1:A:193:ALA:HA	1:A:217:ASN:HB3	1.84	0.58
1:A:88:LEU:HA	1:A:112:ASN:HB3	1.86	0.57
1:A:550:GLY:CA	1:A:556:LYS:HB2	2.33	0.57
1:A:184:VAL:HA	1:A:189:LEU:O	2.04	0.57
1:A:81:ARG:HG3	1:A:82:SER:N	2.18	0.57
1:A:15:ARG:HD2	1:A:16:CGU:OE22	2.05	0.57
1:A:169:GLN:O	1:A:170:CYS:CB	2.53	0.56
1:A:16:CGU:HA	1:A:20:CGU:OE11	2.06	0.56
1:A:511:LYS:HG2	1:A:557:TYR:OH	2.05	0.56
1:A:116:ASN:ND2	1:A:123:GLY:HA2	2.20	0.56
1:A:79:ILE:HG23	1:A:80:THR:N	2.20	0.56
1:A:376:GLU:HG2	1:A:403:LYS:HA	1.88	0.56
1:A:37:THR:O	1:A:38:ASP:HB2	2.06	0.56
1:A:193:ALA:CA	1:A:217:ASN:HB3	2.35	0.56
1:A:563:VAL:HB	1:A:566:LEU:HD12	1.88	0.56
1:A:114:CYS:HA	1:A:125:TRP:O	2.07	0.55
1:A:341:LYS:HD2	1:A:377:ASN:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:PHE:HB3	1:A:222:PRO:HB2	1.87	0.55
1:A:305:GLU:HG3	1:A:309:GLU:CG	2.37	0.55
1:A:48:GLU:C	1:A:50:ALA:H	2.09	0.55
1:A:449:LEU:HD21	1:A:533:SER:HB2	1.87	0.55
1:A:194:TRP:O	1:A:200:LYS:HG2	2.07	0.55
1:A:337:MET:HE2	1:A:346:LEU:CD1	2.37	0.54
1:A:74:ARG:HD2	1:A:108:ASP:CB	2.36	0.54
1:A:40:PHE:CD1	1:A:43:LYS:HD3	2.43	0.54
1:A:363:HIS:CD2	1:A:468:TRP:HZ2	2.25	0.54
1:A:401:LEU:HD23	1:A:425:LEU:HD23	1.90	0.54
1:A:32:CGU:O	1:A:33:SER:HB3	2.07	0.53
1:A:52:THR:CG2	1:A:53:PRO:HD3	2.39	0.53
1:A:574:ILE:HG13	1:A:575:ASP:H	1.74	0.53
1:A:306:ASP:CG	1:A:309:GLU:HB3	2.29	0.52
1:A:415:ASN:O	1:A:416:LEU:C	2.46	0.52
1:A:563:VAL:O	1:A:563:VAL:HG23	2.08	0.52
1:A:536:ASN:HD22	1:A:536:ASN:N	2.08	0.52
1:A:130:ASP:OD1	1:A:132:THR:OG1	2.29	0.51
1:A:290:GLU:C	1:A:292:ASP:H	2.13	0.50
1:A:125:TRP:HA	1:A:138:CYS:SG	2.51	0.50
1:A:144:GLY:C	1:A:168:GLU:N	2.64	0.50
1:A:541:GLN:HG2	1:A:563:VAL:HG11	1.93	0.50
1:A:220:ARG:HG2	1:A:220:ARG:HH11	1.76	0.50
1:A:442:ASP:OD1	1:A:445:THR:HB	2.12	0.50
1:A:385:LYS:NZ	1:A:390:ARG:O	2.44	0.50
1:A:534:PRO:O	1:A:535:PHE:CD2	2.66	0.49
1:A:290:GLU:O	1:A:292:ASP:N	2.45	0.49
1:A:395:ILE:HG23	1:A:434:TYR:CD2	2.48	0.49
1:A:520:ALA:O	1:A:522:GLU:N	2.46	0.49
1:A:104:HIS:ND1	1:A:117:PRO:HB2	2.28	0.48
1:A:431:PHE:O	1:A:432:SER:HB3	2.13	0.48
1:A:540:TYR:CD1	1:A:540:TYR:N	2.81	0.48
1:A:574:ILE:HG13	1:A:575:ASP:N	2.28	0.48
1:A:194:TRP:CD1	1:A:214:LEU:HB3	2.48	0.48
1:A:124:PRO:CG	1:A:140:ILE:HD13	2.43	0.48
1:A:194:TRP:CH2	1:A:231:CYS:HA	2.49	0.47
1:A:479:VAL:CG1	1:A:480:LEU:N	2.77	0.47
1:A:48:GLU:C	1:A:50:ALA:N	2.67	0.47
1:A:542:MET:C	1:A:563:VAL:HG13	2.34	0.47
1:A:276:GLU:HG2	1:A:277:TYR:N	2.30	0.47
1:A:337:MET:HB2	1:A:382:ARG:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:THR:HG22	1:A:482:VAL:HG23	1.97	0.47
1:A:39:VAL:HG21	1:A:74:ARG:NH2	2.30	0.47
1:A:359:LEU:HD23	1:A:422:LEU:HD12	1.98	0.46
1:A:193:ALA:HA	1:A:217:ASN:CB	2.45	0.46
1:A:185:THR:HA	1:A:243:CYS:HA	1.97	0.46
1:A:198:GLN:O	1:A:203:SER:N	2.48	0.46
1:A:511:LYS:C	1:A:511:LYS:HD3	2.36	0.46
1:A:337:MET:HE2	1:A:346:LEU:HD12	1.98	0.46
1:A:445:THR:HG21	1:A:540:TYR:CE2	2.51	0.46
1:A:420:ILE:HD11	1:A:561:THR:HG21	1.97	0.46
1:A:533:SER:HB3	1:A:536:ASN:HD21	1.81	0.46
1:A:504:ASN:OD1	1:A:565:ARG:HD2	2.16	0.46
1:A:386:HIS:NE2	1:A:479:VAL:CG1	2.78	0.46
1:A:407:HIS:CG	1:A:408:PRO:HD2	2.51	0.46
1:A:225:ASP:OD1	1:A:227:GLU:N	2.43	0.45
1:A:239:ASP:O	1:A:240:PHE:HB3	2.16	0.45
1:A:40:PHE:HD1	1:A:43:LYS:HD3	1.80	0.45
1:A:52:THR:HG23	1:A:53:PRO:CD	2.45	0.45
1:A:440:LEU:O	1:A:567:LYS:HE2	2.17	0.45
1:A:74:ARG:CD	1:A:108:ASP:HB2	2.45	0.45
1:A:233:VAL:HG22	1:A:240:PHE:CA	2.47	0.45
1:A:381:VAL:O	1:A:398:ILE:HA	2.17	0.45
1:A:179:GLN:O	1:A:220:ARG:NH2	2.51	0.44
1:A:396:GLU:O	1:A:396:GLU:HG3	2.17	0.44
1:A:53:PRO:HG2	1:A:55:ASP:OD1	2.18	0.44
1:A:218:PHE:CB	1:A:220:ARG:HH12	2.30	0.44
1:A:368:PRO:HG2	1:A:412:TRP:CZ2	2.52	0.44
1:A:386:HIS:NE2	1:A:479:VAL:HG11	2.32	0.44
1:A:316:TYR:HD1	1:A:317:ILE:HG13	1.83	0.44
1:A:512:PRO:HG3	1:A:518:GLY:HA3	1.99	0.44
1:A:490:ARG:HB3	1:A:491:PRO:HD3	2.00	0.44
1:A:92:ARG:HD3	1:A:96:LYS:HG3	1.98	0.44
1:A:174:ARG:NH1	1:A:565:ARG:HH11	2.16	0.43
1:A:517:ARG:NH2	1:A:519:ASP:HB2	2.32	0.43
1:A:140:ILE:HG22	1:A:141:PRO:O	2.18	0.43
1:A:225:ASP:OD1	1:A:226:GLU:N	2.51	0.43
1:A:418:ARG:CD	1:A:504:ASN:ND2	2.67	0.43
1:A:314:GLU:HB3	1:A:317:ILE:HD12	1.99	0.43
1:A:434:TYR:CD1	1:A:434:TYR:N	2.87	0.43
1:A:418:ARG:NH1	1:A:504:ASN:CB	2.81	0.43
1:A:144:GLY:C	1:A:168:GLU:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:PHE:O	1:A:115:ARG:HG2	2.19	0.42
1:A:290:GLU:C	1:A:292:ASP:N	2.71	0.42
1:A:227:GLU:OE1	1:A:418:ARG:NH2	2.51	0.42
1:A:171:VAL:HA	1:A:172:PRO:HD3	1.82	0.42
1:A:407:HIS:HA	1:A:408:PRO:HD3	1.81	0.42
1:A:389:THR:OG1	1:A:390:ARG:N	2.51	0.42
1:A:324:GLY:HA2	1:A:482:VAL:O	2.19	0.42
1:A:174:ARG:NH1	1:A:565:ARG:NH1	2.67	0.42
1:A:533:SER:HA	1:A:534:PRO:HD3	1.92	0.42
1:A:531:MET:SD	1:A:542:MET:HG3	2.60	0.42
1:A:186:THR:HG21	1:A:409:ARG:HG3	2.02	0.41
1:A:79:ILE:CG2	1:A:80:THR:N	2.82	0.41
1:A:337:MET:CE	1:A:346:LEU:CD1	2.93	0.41
1:A:37:THR:O	1:A:38:ASP:CB	2.66	0.41
1:A:171:VAL:O	1:A:247:TYR:HA	2.20	0.41
1:A:391:TYR:C	1:A:391:TYR:CD1	2.94	0.41
1:A:382:ARG:NH2	1:A:396:GLU:OE2	2.47	0.41
1:A:124:PRO:HG2	1:A:140:ILE:HD13	2.02	0.41
1:A:128:THR:HB	1:A:133:VAL:O	2.20	0.41
1:A:236:LYS:O	1:A:239:ASP:HB2	2.21	0.41
1:A:402:GLU:HB2	1:A:426:LYS:HA	2.01	0.41
1:A:130:ASP:HA	1:A:131:PRO:HD3	1.89	0.41
1:A:441:PRO:HB3	1:A:540:TYR:HD2	1.86	0.41
1:A:334:TRP:CD2	1:A:438:VAL:HG23	2.56	0.41
1:A:71:THR:HG21	1:A:119:SER:OG	2.21	0.41
1:A:174:ARG:HH22	1:A:418:ARG:HH22	1.69	0.41
1:A:199:ALA:O	1:A:203:SER:HB3	2.21	0.41
1:A:485:LEU:HD22	1:A:509:GLY:HA2	2.02	0.41
1:A:568:LYS:CA	1:A:571:GLN:HB2	2.40	0.40
1:A:568:LYS:O	1:A:572:LYS:HE2	2.21	0.40
1:A:77:VAL:HG21	1:A:140:ILE:HG13	2.03	0.40
1:A:359:LEU:HD23	1:A:359:LEU:HA	1.83	0.40
1:A:74:ARG:NH1	1:A:108:ASP:H	2.19	0.40

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	525/557 (94%)	412 (78%)	88 (17%)	25 (5%)	2	16

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	33	SER
1	A	38	ASP
1	A	52	THR
1	A	63	GLY
1	A	195	ALA
1	A	321	ILE
1	A	432	SER
1	A	5	LEU
1	A	49	THR
1	A	180	GLY
1	A	291	ALA
1	A	403	LYS
1	A	35	THR
1	A	239	ASP
1	A	376	GLU
1	A	498	ARG
1	A	537	ASN
1	A	51	ARG
1	A	318	ASP
1	A	414	GLU
1	A	536	ASN
1	A	83	GLY
1	A	534	PRO
1	A	222	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	452/466 (97%)	373 (82%)	79 (18%)	<b>2</b> <b>8</b>

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	TYR
1	A	31	LEU
1	A	37	THR
1	A	38	ASP
1	A	39	VAL
1	A	41	TRP
1	A	55	ASP
1	A	61	LEU
1	A	71	THR
1	A	72	ASN
1	A	79	ILE
1	A	81	ARG
1	A	98	GLU
1	A	110	GLN
1	A	126	CYS
1	A	129	THR
1	A	135	ARG
1	A	142	VAL
1	A	171	VAL
1	A	176	GLN
1	A	177	GLN
1	A	179	GLN
1	A	186	THR
1	A	192	LEU
1	A	198	GLN
1	A	204	LYS
1	A	239	ASP
1	A	249	GLU
1	A	275	SER
1	A	276	GLU

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Mol	Chain	Res	Type
1	A	279	THR
1	A	303	SER
1	A	306	ASP
1	A	309	GLU
1	A	311	GLU
1	A	312	LEU
1	A	313	LEU
1	A	316	TYR
1	A	332	SER
1	A	334	TRP
1	A	339	PHE
1	A	340	ARG
1	A	344	GLN
1	A	345	GLU
1	A	346	LEU
1	A	356	ARG
1	A	359	LEU
1	A	366	LEU
1	A	378	ASP
1	A	382	ARG
1	A	394	ASN
1	A	396	GLU
1	A	397	LYS
1	A	398	ILE
1	A	403	LYS
1	A	415	ASN
1	A	433	ASP
1	A	438	VAL
1	A	442	ASP
1	A	443	ARG
1	A	465	LYS
1	A	469	THR
1	A	472	VAL
1	A	474	LYS
1	A	476	GLN
1	A	478	SER
1	A	488	VAL
1	A	492	VAL
1	A	494	LYS
1	A	499	ILE
1	A	502	THR
1	A	510	TYR

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Mol	Chain	Res	Type
1	A	511	LYS
1	A	525	SER
1	A	536	ASN
1	A	554	ASP
1	A	571	GLN
1	A	573	VAL
1	A	575	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	176	GLN
1	A	179	GLN
1	A	377	ASN
1	A	394	ASN
1	A	415	ASN
1	A	504	ASN
1	A	536	ASN
1	A	537	ASN

### 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	26	1,2	3,11,12	0.85	0	1,14,16	0.30	0
1	CGU	A	14	1	3,11,12	0.61	0	1,14,16	0.82	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CGU	A	6	1,2	3,11,12	0.84	0	1,14,16	0.29	0
1	CGU	A	19	1	3,11,12	0.66	0	1,14,16	0.45	0
1	CGU	A	16	1,2	3,11,12	1.01	0	1,14,16	0.21	0
1	CGU	A	7	1,2	3,11,12	0.68	0	1,14,16	0.47	0
1	CGU	A	32	1	3,11,12	0.75	0	1,14,16	0.53	0
1	CGU	A	29	1,2	3,11,12	0.60	0	1,14,16	0.58	0
1	CGU	A	20	1,2	3,11,12	0.48	0	1,14,16	0.05	0
1	CGU	A	25	1	3,11,12	0.84	0	1,14,16	0.92	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	26	1,2	-	3/5/14/16	-
1	CGU	A	14	1	-	0/5/14/16	-
1	CGU	A	6	1,2	-	4/5/14/16	-
1	CGU	A	19	1	-	3/5/14/16	-
1	CGU	A	16	1,2	-	0/5/14/16	-
1	CGU	A	7	1,2	-	1/5/14/16	-
1	CGU	A	32	1	-	1/5/14/16	-
1	CGU	A	29	1,2	-	0/5/14/16	-
1	CGU	A	20	1,2	-	3/5/14/16	-
1	CGU	A	25	1	-	2/5/14/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	26	CGU	N-CA-CB-CG
1	A	6	CGU	O-C-CA-CB
1	A	19	CGU	O-C-CA-CB
1	A	7	CGU	O-C-CA-CB
1	A	32	CGU	N-CA-CB-CG
1	A	25	CGU	O-C-CA-CB
1	A	25	CGU	C-CA-CB-CG
1	A	26	CGU	CA-CB-CG-CD1

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Mol	Chain	Res	Type	Atoms
1	A	20	CGU	CA-CB-CG-CD2
1	A	20	CGU	CA-CB-CG-CD1
1	A	6	CGU	CA-CB-CG-CD1
1	A	26	CGU	C-CA-CB-CG
1	A	6	CGU	CA-CB-CG-CD2
1	A	19	CGU	C-CA-CB-CG
1	A	6	CGU	N-CA-CB-CG
1	A	20	CGU	N-CA-CB-CG
1	A	19	CGU	CA-CB-CG-CD2

There are no ring outliers.

6 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	14	CGU	1	0
1	A	19	CGU	1	0
1	A	16	CGU	2	0
1	A	7	CGU	1	0
1	A	32	CGU	1	0
1	A	20	CGU	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 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	701	1	14,14,15	0.80	1 (7%)	17,19,21	1.97	3 (17%)
3	NAG	A	703	1	14,14,15	1.18	1 (7%)	17,19,21	1.99	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	702	1	14,14,15	0.59	0	17,19,21	1.19	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
3	NAG	A	701	1	-	0/6/23/26	0/1/1/1
3	NAG	A	703	1	-	2/6/23/26	0/1/1/1
3	NAG	A	702	1	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	703	NAG	C1-C2	3.45	1.57	1.52
3	A	701	NAG	C1-C2	2.17	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	703	NAG	C2-N2-C7	4.86	129.83	122.90
3	A	701	NAG	C4-C3-C2	4.55	117.68	111.02
3	A	701	NAG	C1-O5-C5	4.21	117.90	112.19
3	A	701	NAG	O5-C5-C6	3.18	112.19	107.20
3	A	703	NAG	C4-C3-C2	3.05	115.49	111.02
3	A	703	NAG	O5-C5-C4	-3.04	103.43	110.83
3	A	703	NAG	O7-C7-C8	-2.51	117.40	122.06
3	A	703	NAG	O7-C7-N2	2.42	126.40	121.95
3	A	702	NAG	O5-C1-C2	-2.39	107.52	111.29
3	A	702	NAG	C1-O5-C5	2.19	115.15	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	703	NAG	C4-C5-C6-O6
3	A	703	NAG	O5-C5-C6-O6
3	A	702	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	529/557 (94%)	-0.19	5 (0%) 84 88	37, 68, 106, 128	1 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	202	LEU	3.3
1	A	38	ASP	3.2
1	A	578	GLY	2.9
1	A	68	GLY	2.1
1	A	201	ALA	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains

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(Å <sup>2</sup> )	Q<0.9
1	CGU	A	32	12/13	0.68	0.38	122,123,123,123	0
1	CGU	A	19	12/13	0.84	0.12	101,102,103,103	0
1	CGU	A	25	12/13	0.88	0.11	108,109,110,110	0
1	CGU	A	29	12/13	0.90	0.14	108,111,114,114	0
1	CGU	A	20	12/13	0.90	0.12	99,101,103,103	0
1	CGU	A	14	12/13	0.90	0.14	97,103,105,105	0
1	CGU	A	6	12/13	0.91	0.21	94,98,100,102	0
1	CGU	A	26	12/13	0.91	0.17	103,107,110,110	0
1	CGU	A	7	12/13	0.95	0.14	98,99,100,100	0
1	CGU	A	16	12/13	0.96	0.15	95,98,101,101	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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	CA	A	606	1/1	0.77	0.22	68,68,68,68	0
3	NAG	A	703	14/15	0.84	0.15	88,90,92,92	0
3	NAG	A	701	14/15	0.85	0.16	73,77,78,79	0
3	NAG	A	702	14/15	0.87	0.17	88,90,91,91	0
2	CA	A	602	1/1	0.95	0.29	100,100,100,100	0
2	CA	A	604	1/1	0.95	0.22	97,97,97,97	0
2	CA	A	603	1/1	0.96	0.25	86,86,86,86	0
2	CA	A	605	1/1	0.96	0.19	101,101,101,101	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.