



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:28 AM UTC

PDB ID : 2PF2 / pdb_00002pf2
Title : THE CA²⁺ ION AND MEMBRANE BINDING STRUCTURE OF THE GLA DOMAIN OF CA-PROTHROMBIN FRAGMENT 1
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Deposited on : 1991-12-08
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

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>.

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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

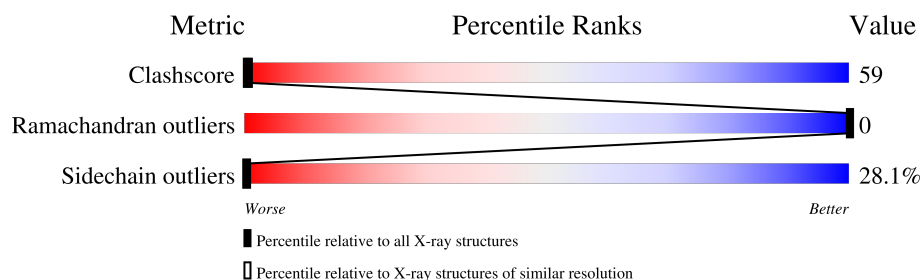
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	156	16% 41% 32% • 6%

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
1	CGU	A	26	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1317 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 FRAGMENT 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	0	0	1
			1166	701	208	246	11			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	CGU	GLU	conflict	UNP P00735
A	8	CGU	GLU	conflict	UNP P00735
A	15	CGU	GLU	conflict	UNP P00735
A	17	CGU	GLU	conflict	UNP P00735
A	20	CGU	GLU	conflict	UNP P00735
A	21	CGU	GLU	conflict	UNP P00735
A	26	CGU	GLU	conflict	UNP P00735
A	27	CGU	GLU	conflict	UNP P00735
A	30	CGU	GLU	conflict	UNP P00735
A	33	CGU	GLU	conflict	UNP P00735

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is water.

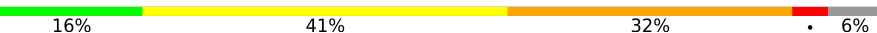
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	144	Total	O	0	0
			144	144		

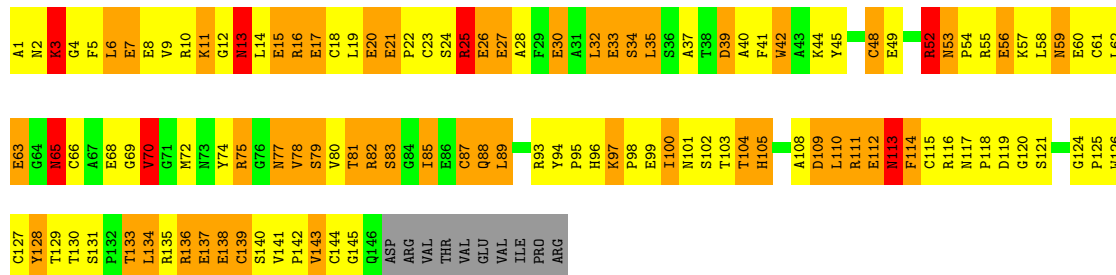
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

• Molecule 1: PROTHROMBIN FRAGMENT 1

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	39.39Å 53.88Å 129.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT, PROLSQ, X-PLOR	Depositor
R, R_{free}	0.171 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1317	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

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

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	1.23	4/1063 (0.4%)	2.54	82/1428 (5.7%)

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	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	GLY	C-N	-6.42	1.24	1.33
1	A	139	CYS	CA-C	5.87	1.59	1.52
1	A	4	GLY	C-N	-5.75	1.25	1.33
1	A	69	GLY	C-N	-5.21	1.27	1.34

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ASN	OD1-CG-ND2	11.53	134.13	122.60
1	A	13	ASN	CA-C-O	-9.99	108.25	120.54
1	A	79	SER	N-CA-CB	-9.77	96.88	110.95
1	A	105	HIS	CA-CB-CG	9.24	123.04	113.80
1	A	119	ASP	CA-CB-CG	9.23	121.83	112.60
1	A	12	GLY	CA-C-O	-9.15	110.34	122.24
1	A	113	ASN	CA-C-N	8.98	134.34	121.50
1	A	113	ASN	C-N-CA	8.98	134.34	121.50
1	A	93	ARG	CA-CB-CG	8.75	131.60	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	LEU	CA-C-O	-8.45	111.86	121.15
1	A	87	CYS	CA-C-N	8.44	132.86	120.87
1	A	87	CYS	C-N-CA	8.44	132.86	120.87
1	A	127	CYS	CA-C-O	-8.37	112.32	121.28
1	A	42	TRP	CA-C-N	8.37	131.82	120.44
1	A	42	TRP	C-N-CA	8.37	131.82	120.44
1	A	3	LYS	N-CA-CB	-8.36	101.76	111.79
1	A	88	GLN	OE1-CD-NE2	-7.95	114.66	122.60
1	A	37	ALA	CA-C-N	7.89	134.07	120.58
1	A	37	ALA	C-N-CA	7.89	134.07	120.58
1	A	13	ASN	CA-CB-CG	7.61	120.21	112.60
1	A	105	HIS	CA-C-N	7.50	127.13	119.56
1	A	105	HIS	C-N-CA	7.50	127.13	119.56
1	A	57	LYS	N-CA-C	-7.42	103.18	112.90
1	A	77	ASN	CA-CB-CG	7.42	120.02	112.60
1	A	70	VAL	CA-CB-CG1	7.35	122.90	110.40
1	A	35	LEU	CA-C-O	7.30	128.37	119.97
1	A	89	LEU	O-C-N	7.26	131.82	122.97
1	A	65	ASN	CA-CB-CG	-7.17	105.42	112.60
1	A	121	SER	N-CA-C	-7.13	99.89	110.23
1	A	56	GLU	N-CA-C	-7.08	104.45	113.23
1	A	25	ARG	CD-NE-CZ	6.95	134.13	124.40
1	A	109	ASP	CA-CB-CG	6.93	119.53	112.60
1	A	88	GLN	CG-CD-OE1	6.93	134.65	120.80
1	A	12	GLY	O-C-N	6.87	131.96	122.82
1	A	80	VAL	O-C-N	6.83	130.10	123.14
1	A	85	ILE	CA-C-O	-6.72	112.71	120.98
1	A	131	SER	CA-C-O	6.70	125.42	119.59
1	A	39	ASP	N-CA-C	-6.67	103.93	111.07
1	A	12	GLY	N-CA-C	-6.53	105.14	112.33
1	A	13	ASN	O-C-N	6.48	131.00	123.41
1	A	133	THR	N-CA-C	6.40	120.83	112.89
1	A	81	THR	CA-C-N	6.33	129.28	120.29
1	A	81	THR	C-N-CA	6.33	129.28	120.29
1	A	93	ARG	O-C-N	6.33	129.85	122.19
1	A	77	ASN	OD1-CG-ND2	-6.30	116.30	122.60
1	A	85	ILE	CB-CA-C	-6.26	101.92	111.69
1	A	14	LEU	CB-CA-C	6.26	121.99	110.10
1	A	52	ARG	CD-NE-CZ	6.21	133.09	124.40
1	A	128	TYR	N-CA-CB	6.12	120.14	110.23
1	A	39	ASP	CA-C-O	-6.07	114.44	120.82
1	A	121	SER	CB-CA-C	6.00	119.68	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	LYS	N-CA-C	5.98	117.47	110.41
1	A	16	ARG	NE-CZ-NH2	5.98	124.58	119.20
1	A	114	PHE	CA-CB-CG	5.97	119.77	113.80
1	A	58	LEU	N-CA-C	-5.93	104.17	111.40
1	A	102	SER	N-CA-C	5.88	119.28	111.75
1	A	93	ARG	CA-C-O	-5.86	112.57	119.48
1	A	108	ALA	CB-CA-C	5.84	121.65	109.68
1	A	39	ASP	N-CA-CB	5.84	118.47	110.01
1	A	11	LYS	O-C-N	5.80	130.07	122.93
1	A	78	VAL	N-CA-CB	5.74	117.88	110.99
1	A	35	LEU	N-CA-C	-5.71	105.20	111.82
1	A	121	SER	CA-CB-OG	5.62	122.35	111.10
1	A	94	TYR	O-C-N	5.58	127.80	121.94
1	A	127	CYS	O-C-N	5.55	128.84	123.29
1	A	56	GLU	N-CA-CB	5.54	119.09	110.44
1	A	145	GLY	O-C-N	5.50	131.81	123.00
1	A	69	GLY	CA-C-N	5.45	130.08	121.09
1	A	69	GLY	C-N-CA	5.45	130.08	121.09
1	A	56	GLU	CA-C-O	5.44	125.63	119.27
1	A	34	SER	CA-CB-OG	5.43	121.95	111.10
1	A	39	ASP	O-C-N	5.42	127.66	122.07
1	A	105	HIS	O-C-N	5.42	125.15	121.19
1	A	23	CYS	CA-CB-SG	5.24	126.45	114.40
1	A	48	CYS	CA-C-O	5.21	125.74	119.59
1	A	145	GLY	CA-C-O	-5.19	109.90	120.80
1	A	130	THR	CB-CA-C	5.12	120.84	110.38
1	A	18	CYS	CA-C-O	-5.12	112.09	120.80
1	A	13	ASN	OD1-CG-ND2	-5.02	117.58	122.60
1	A	40	ALA	CA-C-N	5.01	131.10	121.54
1	A	40	ALA	C-N-CA	5.01	131.10	121.54
1	A	121	SER	CA-C-O	-5.00	115.69	121.19

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	ASN	Mainchain
1	A	70	VAL	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1166	0	1042	129	0
2	A	7	0	0	0	0
3	A	144	0	0	15	0
All	All	1317	0	1042	129	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 59.

All (129) 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:104:THR:CG2	1:A:105:HIS:HD2	1.49	1.23
1:A:104:THR:HG23	1:A:105:HIS:CD2	1.84	1.11
1:A:104:THR:HG23	1:A:105:HIS:HD2	1.12	1.09
1:A:82:ARG:NH2	1:A:140:SER:HB3	1.68	1.06
1:A:104:THR:CG2	1:A:105:HIS:CD2	2.40	1.04
1:A:138:GLU:HB3	3:A:305:HOH:O	1.56	1.04
1:A:135:ARG:HG2	1:A:136:ARG:HG3	1.43	0.97
1:A:79:SER:O	1:A:87:CYS:SG	2.21	0.96
1:A:82:ARG:HH12	1:A:140:SER:HA	1.30	0.95
1:A:96:HIS:O	1:A:98:PRO:HD3	1.67	0.94
1:A:104:THR:HG22	1:A:105:HIS:HD2	1.34	0.92
1:A:117:ASN:OD1	1:A:120:GLY:N	2.03	0.91
1:A:113:ASN:HD22	1:A:113:ASN:H	1.16	0.88
1:A:16:ARG:NH1	3:A:190:HOH:O	2.11	0.84
1:A:129:THR:OG1	1:A:134:LEU:O	1.97	0.82
1:A:109:ASP:OD1	1:A:111:ARG:HD3	1.81	0.81
1:A:25:ARG:NH2	1:A:39:ASP:OD1	2.17	0.78
1:A:15:CGU:O	1:A:20:CGU:HB3	1.84	0.77
1:A:75:ARG:C	1:A:116:ARG:NH2	2.44	0.75
1:A:15:CGU:OE21	1:A:55:ARG:NH2	2.16	0.75
1:A:53:ASN:HA	1:A:54:PRO:C	2.11	0.74
1:A:82:ARG:CZ	1:A:140:SER:HB3	2.17	0.73
1:A:82:ARG:HH22	1:A:140:SER:HB3	1.53	0.73
1:A:55:ARG:O	1:A:55:ARG:HG3	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:CGU:O	1:A:10:ARG:HG2	1.89	0.72
1:A:75:ARG:HG2	3:A:362:HOH:O	1.91	0.71
1:A:59:ASN:HD22	1:A:59:ASN:N	1.86	0.70
1:A:113:ASN:HD22	1:A:113:ASN:N	1.89	0.69
1:A:115:CYS:HA	1:A:126:TRP:O	1.93	0.69
1:A:82:ARG:HD2	1:A:138:GLU:HG2	1.73	0.68
1:A:5:PHE:CE1	1:A:6:LEU:HD22	2.30	0.67
1:A:82:ARG:NH1	1:A:140:SER:HA	2.05	0.67
1:A:138:GLU:CB	3:A:305:HOH:O	2.26	0.67
1:A:82:ARG:HD3	1:A:138:GLU:OE2	1.95	0.66
1:A:82:ARG:NH2	1:A:140:SER:CB	2.54	0.66
1:A:138:GLU:CG	3:A:305:HOH:O	2.43	0.65
1:A:59:ASN:HB2	3:A:188:HOH:O	1.97	0.64
1:A:82:ARG:HH12	1:A:140:SER:CA	2.08	0.64
1:A:82:ARG:HD3	1:A:138:GLU:CD	2.23	0.64
1:A:70:VAL:O	1:A:124:GLY:HA2	1.98	0.63
1:A:82:ARG:CD	1:A:138:GLU:HG2	2.28	0.63
1:A:83:SER:HB2	1:A:85:ILE:HG13	1.80	0.63
1:A:75:ARG:HA	1:A:116:ARG:NH2	2.13	0.63
1:A:77:ASN:OD1	3:A:277:HOH:O	2.16	0.62
1:A:82:ARG:HH22	1:A:140:SER:CB	2.12	0.62
1:A:113:ASN:H	1:A:113:ASN:ND2	1.94	0.61
1:A:1:ALA:O	1:A:2:ASN:HB2	2.00	0.61
1:A:104:THR:HG22	1:A:105:HIS:CD2	2.20	0.60
1:A:85:ILE:HD12	1:A:134:LEU:HD12	1.83	0.59
1:A:3:LYS:N	1:A:7:CGU:OE12	2.29	0.59
1:A:11:LYS:O	1:A:16:ARG:NH2	2.35	0.59
1:A:99:GLU:N	1:A:99:GLU:OE1	2.36	0.58
1:A:74:TYR:O	3:A:242:HOH:O	2.17	0.58
1:A:16:ARG:HA	1:A:20:CGU:OE11	2.02	0.57
1:A:109:ASP:OD1	1:A:111:ARG:CD	2.50	0.57
1:A:87:CYS:HB2	1:A:113:ASN:O	2.05	0.57
1:A:63:GLU:HG3	3:A:249:HOH:O	2.05	0.56
1:A:75:ARG:CA	1:A:116:ARG:NH2	2.68	0.56
1:A:101:ASN:C	1:A:101:ASN:OD1	2.49	0.55
1:A:33:CGU:O	1:A:34:SER:C	2.49	0.55
1:A:98:PRO:HB3	1:A:128:TYR:CE1	2.41	0.54
1:A:24:SER:OG	1:A:27:CGU:HG	2.07	0.54
1:A:82:ARG:NH1	1:A:140:SER:CA	2.68	0.54
1:A:143:VAL:HG12	3:A:196:HOH:O	2.06	0.54
1:A:85:ILE:HG21	1:A:129:THR:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ARG:HD2	1:A:17:CGU:OE22	2.09	0.53
1:A:74:TYR:CD1	1:A:141:VAL:HG11	2.43	0.52
1:A:134:LEU:HD11	1:A:137:GLU:HG3	1.90	0.52
1:A:44:LYS:HE2	1:A:75:ARG:HD2	1.92	0.52
1:A:81:THR:HB	1:A:137:GLU:OE1	2.10	0.52
1:A:99:GLU:H	1:A:99:GLU:CD	2.18	0.52
1:A:83:SER:OG	1:A:137:GLU:OE2	2.28	0.51
1:A:5:PHE:O	1:A:6:LEU:HB2	2.11	0.51
1:A:41:PHE:O	1:A:42:TRP:C	2.54	0.51
1:A:20:CGU:OE11	1:A:20:CGU:OE21	2.23	0.50
1:A:117:ASN:OD1	1:A:120:GLY:CA	2.59	0.50
1:A:82:ARG:NH1	1:A:139:CYS:C	2.70	0.50
1:A:75:ARG:C	1:A:116:ARG:HH21	2.21	0.49
1:A:82:ARG:HD2	1:A:138:GLU:CG	2.42	0.49
1:A:100:ILE:HG21	1:A:118:PRO:HG2	1.95	0.49
1:A:135:ARG:CG	1:A:136:ARG:HG3	2.31	0.48
1:A:42:TRP:CZ3	1:A:45:TYR:CE2	3.01	0.48
1:A:62:LEU:O	3:A:204:HOH:O	2.20	0.48
1:A:68:GLU:HB2	1:A:144:CYS:SG	2.53	0.48
1:A:88:GLN:HG3	1:A:95:PRO:HD2	1.96	0.48
1:A:32:LEU:HD12	1:A:32:LEU:HA	1.73	0.47
1:A:82:ARG:HB2	1:A:138:GLU:O	2.15	0.47
1:A:55:ARG:O	1:A:55:ARG:CG	2.60	0.46
1:A:88:GLN:OE1	1:A:96:HIS:O	2.33	0.46
1:A:82:ARG:NH1	1:A:139:CYS:O	2.48	0.46
1:A:85:ILE:CD1	1:A:134:LEU:HD12	2.46	0.46
1:A:112:GLU:HB2	1:A:114:PHE:CE2	2.50	0.46
1:A:82:ARG:CD	1:A:138:GLU:CG	2.93	0.46
1:A:97:LYS:HB2	1:A:97:LYS:HE2	1.61	0.46
1:A:59:ASN:N	1:A:59:ASN:ND2	2.60	0.45
1:A:96:HIS:CE1	1:A:135:ARG:HA	2.51	0.45
1:A:111:ARG:O	1:A:112:GLU:C	2.58	0.45
1:A:111:ARG:NH1	3:A:277:HOH:O	2.49	0.45
1:A:28:ALA:O	1:A:32:LEU:HD22	2.17	0.45
1:A:141:VAL:HG13	1:A:142:PRO:HD2	1.99	0.45
1:A:116:ARG:O	1:A:117:ASN:CB	2.65	0.44
1:A:65:ASN:HB2	3:A:182:HOH:O	2.17	0.44
1:A:81:THR:CB	1:A:137:GLU:OE1	2.66	0.44
1:A:13:ASN:O	1:A:17:CGU:HB3	2.17	0.44
1:A:110:LEU:O	3:A:267:HOH:O	2.21	0.43
1:A:16:ARG:O	1:A:21:CGU:OE21	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:CGU:HB2	1:A:22:PRO:HD2	2.00	0.43
1:A:60:GLU:HG2	1:A:66:CYS:SG	2.59	0.42
1:A:112:GLU:HB3	1:A:113:ASN:H	1.39	0.42
1:A:9:VAL:O	1:A:9:VAL:HG12	2.18	0.42
1:A:48:CYS:SG	1:A:61:CYS:C	3.02	0.42
1:A:52:ARG:HH11	1:A:52:ARG:HG3	1.85	0.42
1:A:112:GLU:HB3	1:A:113:ASN:HD22	1.84	0.42
1:A:74:TYR:CE1	1:A:141:VAL:HG11	2.55	0.42
1:A:49:GLU:O	1:A:49:GLU:HG3	2.20	0.41
1:A:85:ILE:CG2	1:A:129:THR:HB	2.50	0.41
1:A:15:CGU:O	1:A:16:ARG:C	2.63	0.41
1:A:42:TRP:CZ3	1:A:45:TYR:CD2	3.07	0.41
1:A:9:VAL:O	1:A:9:VAL:CG1	2.68	0.41
1:A:53:ASN:HA	1:A:54:PRO:O	2.20	0.41
1:A:99:GLU:OE1	1:A:135:ARG:NH1	2.51	0.41
1:A:117:ASN:HB2	1:A:125:PRO:HA	2.02	0.41
1:A:15:CGU:OE21	1:A:15:CGU:OE12	2.37	0.41
1:A:19:LEU:O	1:A:55:ARG:NH1	2.54	0.40
1:A:26:CGU:HB3	3:A:240:HOH:O	2.20	0.40
1:A:26:CGU:O	1:A:30:CGU:HG	2.22	0.40
1:A:110:LEU:HD12	1:A:116:ARG:HG3	2.02	0.40
1:A:44:LYS:O	1:A:62:LEU:HD23	2.21	0.40
1:A:16:ARG:O	1:A:20:CGU:HB2	2.21	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	134/156 (86%)	115 (86%)	19 (14%)	0	100	100

There are no Ramachandran outliers to report.

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	114/125 (91%)	82 (72%)	32 (28%)	0 0

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	6	LEU
1	A	25	ARG
1	A	32	LEU
1	A	35	LEU
1	A	52	ARG
1	A	53	ASN
1	A	56	GLU
1	A	59	ASN
1	A	63	GLU
1	A	65	ASN
1	A	70	VAL
1	A	72	MET
1	A	75	ARG
1	A	78	VAL
1	A	82	ARG
1	A	83	SER
1	A	89	LEU
1	A	97	LYS
1	A	100	ILE
1	A	103	THR
1	A	104	THR
1	A	110	LEU
1	A	111	ARG
1	A	112	GLU
1	A	113	ASN
1	A	133	THR
1	A	134	LEU
1	A	136	ARG
1	A	137	GLU

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Mol	Chain	Res	Type
1	A	138	GLU
1	A	143	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	65	ASN
1	A	77	ASN
1	A	105	HIS
1	A	113	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	21	1,2	9,11,12	1.11	1 (11%)	10,14,16	1.53	2 (20%)
1	CGU	A	20	1,2	9,11,12	1.15	1 (11%)	10,14,16	2.20	4 (40%)
1	CGU	A	8	1,2	9,11,12	0.90	0	10,14,16	2.58	5 (50%)
1	CGU	A	30	1,2	9,11,12	1.33	2 (22%)	10,14,16	1.75	3 (30%)
1	CGU	A	7	1,2	9,11,12	1.03	1 (11%)	10,14,16	1.81	3 (30%)
1	CGU	A	33	1	9,11,12	1.93	2 (22%)	10,14,16	1.98	3 (30%)
1	CGU	A	17	1,2	9,11,12	1.24	0	10,14,16	3.50	6 (60%)
1	CGU	A	15	1,2	9,11,12	1.30	0	10,14,16	1.32	2 (20%)
1	CGU	A	26	1,2	9,11,12	1.33	1 (11%)	10,14,16	2.50	5 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CGU	A	27	1,2	9,11,12	0.82	0	10,14,16	1.31	2 (20%)

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	21	1,2	-	5/13/14/16	-
1	CGU	A	20	1,2	-	5/13/14/16	-
1	CGU	A	8	1,2	-	8/13/14/16	-
1	CGU	A	30	1,2	-	1/13/14/16	-
1	CGU	A	7	1,2	-	8/13/14/16	-
1	CGU	A	33	1	-	3/13/14/16	-
1	CGU	A	17	1,2	-	4/13/14/16	-
1	CGU	A	15	1,2	-	3/13/14/16	-
1	CGU	A	26	1,2	-	11/13/14/16	-
1	CGU	A	27	1,2	-	4/13/14/16	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	33	CGU	OE21-CD2	4.18	1.34	1.22
1	A	33	CGU	OE22-CD2	-3.52	1.19	1.30
1	A	30	CGU	CB-CG	-2.58	1.47	1.54
1	A	20	CGU	OE22-CD2	-2.22	1.23	1.30
1	A	30	CGU	OE12-CD1	-2.11	1.23	1.30
1	A	21	CGU	OE22-CD2	-2.11	1.23	1.30
1	A	26	CGU	O-C	2.04	1.27	1.20
1	A	7	CGU	OE22-CD2	-2.03	1.24	1.30

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	CGU	OE12-CD1-OE11	-5.86	110.78	124.08
1	A	8	CGU	OE11-CD1-CG	5.02	136.93	120.19
1	A	17	CGU	CB-CG-CD1	4.81	122.88	113.11
1	A	33	CGU	CB-CA-C	4.70	118.22	110.99
1	A	17	CGU	CB-CA-N	-4.64	100.35	110.48
1	A	20	CGU	CB-CG-CD1	-4.60	103.76	113.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	CGU	OE12-CD1-OE11	-4.40	114.09	124.08
1	A	17	CGU	CB-CA-C	4.35	117.69	110.99
1	A	8	CGU	OE12-CD1-OE11	-4.22	114.51	124.08
1	A	17	CGU	CB-CG-CD2	-3.60	105.80	113.11
1	A	20	CGU	CB-CA-N	-3.58	102.66	110.48
1	A	26	CGU	CB-CG-CD2	-3.56	105.89	113.11
1	A	26	CGU	OE11-CD1-CG	3.24	130.99	120.19
1	A	15	CGU	CB-CG-CD2	-3.05	106.93	113.11
1	A	26	CGU	CB-CA-C	3.04	115.66	110.99
1	A	7	CGU	OE22-CD2-OE21	-2.95	117.39	124.08
1	A	21	CGU	CB-CG-CD2	-2.86	107.30	113.11
1	A	30	CGU	OE12-CD1-CG	2.72	125.77	116.50
1	A	27	CGU	OE22-CD2-OE21	2.70	130.20	124.08
1	A	7	CGU	CB-CG-CD2	2.59	118.38	113.11
1	A	33	CGU	OE22-CD2-CG	2.50	125.01	116.50
1	A	33	CGU	OE21-CD2-CG	-2.46	111.98	120.19
1	A	17	CGU	OE12-CD1-CG	2.43	124.76	116.50
1	A	30	CGU	OE12-CD1-OE11	-2.42	118.59	124.08
1	A	8	CGU	OE12-CD1-CG	-2.36	108.48	116.50
1	A	26	CGU	CB-CA-N	-2.29	105.47	110.48
1	A	8	CGU	OE21-CD2-CG	2.27	127.76	120.19
1	A	21	CGU	OE22-CD2-CG	-2.26	108.80	116.50
1	A	7	CGU	CB-CA-C	2.26	114.47	110.99
1	A	20	CGU	OE21-CD2-CG	-2.25	112.69	120.19
1	A	8	CGU	CB-CA-N	-2.19	105.70	110.48
1	A	30	CGU	CB-CA-C	-2.17	107.64	110.99
1	A	27	CGU	CB-CA-N	-2.13	105.83	110.48
1	A	15	CGU	CB-CG-CD1	2.06	117.30	113.11
1	A	20	CGU	OE22-CD2-CG	2.03	123.40	116.50

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	7	CGU	O-C-CA-CB
1	A	7	CGU	N-CA-CB-CG
1	A	7	CGU	C-CA-CB-CG
1	A	7	CGU	CA-CB-CG-CD1
1	A	7	CGU	CA-CB-CG-CD2
1	A	8	CGU	N-CA-CB-CG
1	A	8	CGU	C-CA-CB-CG
1	A	8	CGU	CA-CB-CG-CD2

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Mol	Chain	Res	Type	Atoms
1	A	15	CGU	N-CA-CB-CG
1	A	15	CGU	C-CA-CB-CG
1	A	17	CGU	C-CA-CB-CG
1	A	17	CGU	CA-CB-CG-CD2
1	A	20	CGU	OE12-CD1-CG-CD2
1	A	21	CGU	CA-CB-CG-CD1
1	A	21	CGU	CA-CB-CG-CD2
1	A	26	CGU	O-C-CA-CB
1	A	26	CGU	CA-CB-CG-CD1
1	A	26	CGU	OE12-CD1-CG-CD2
1	A	26	CGU	OE22-CD2-CG-CD1
1	A	30	CGU	O-C-CA-CB
1	A	33	CGU	O-C-CA-CB
1	A	27	CGU	CA-CB-CG-CD1
1	A	17	CGU	N-CA-CB-CG
1	A	7	CGU	OE21-CD2-CG-CB
1	A	7	CGU	OE22-CD2-CG-CB
1	A	8	CGU	OE21-CD2-CG-CB
1	A	20	CGU	OE11-CD1-CG-CB
1	A	20	CGU	OE12-CD1-CG-CB
1	A	21	CGU	OE11-CD1-CG-CB
1	A	26	CGU	OE11-CD1-CG-CB
1	A	26	CGU	OE21-CD2-CG-CB
1	A	26	CGU	OE22-CD2-CG-CB
1	A	27	CGU	OE21-CD2-CG-CB
1	A	27	CGU	OE22-CD2-CG-CB
1	A	17	CGU	OE11-CD1-CG-CD2
1	A	20	CGU	OE11-CD1-CG-CD2
1	A	21	CGU	OE11-CD1-CG-CD2
1	A	26	CGU	C-CA-CB-CG
1	A	8	CGU	CA-CB-CG-CD1
1	A	26	CGU	CA-CB-CG-CD2
1	A	20	CGU	N-CA-CB-CG
1	A	26	CGU	N-CA-CB-CG
1	A	8	CGU	OE11-CD1-CG-CB
1	A	8	CGU	OE12-CD1-CG-CB
1	A	8	CGU	OE22-CD2-CG-CB
1	A	33	CGU	OE11-CD1-CG-CB
1	A	33	CGU	OE12-CD1-CG-CB
1	A	7	CGU	OE11-CD1-CG-CD2
1	A	15	CGU	OE21-CD2-CG-CD1
1	A	21	CGU	OE21-CD2-CG-CD1

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Mol	Chain	Res	Type	Atoms
1	A	26	CGU	OE21-CD2-CG-CD1
1	A	27	CGU	OE22-CD2-CG-CD1

There are no ring outliers.

9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	21	CGU	2	0
1	A	20	CGU	4	0
1	A	30	CGU	1	0
1	A	7	CGU	2	0
1	A	33	CGU	1	0
1	A	17	CGU	2	0
1	A	15	CGU	4	0
1	A	26	CGU	2	0
1	A	27	CGU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.