



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2025 – 08:48 AM EDT

PDB ID : 3MMU / pdb\_00003mmu  
Title : Crystal structure of endoglucanase Cel5A from the hyperthermophilic *Thermotoga maritima*  
Authors : Pereira, J.H.; Chen, Z.; McAndrew, R.P.; Sapra, R.; Chhabra, S.R.; Sale, K.L.; Simmons, B.A.; Adams, P.D.  
Deposited on : 2010-04-20  
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

<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 Phenix2.0rc1  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

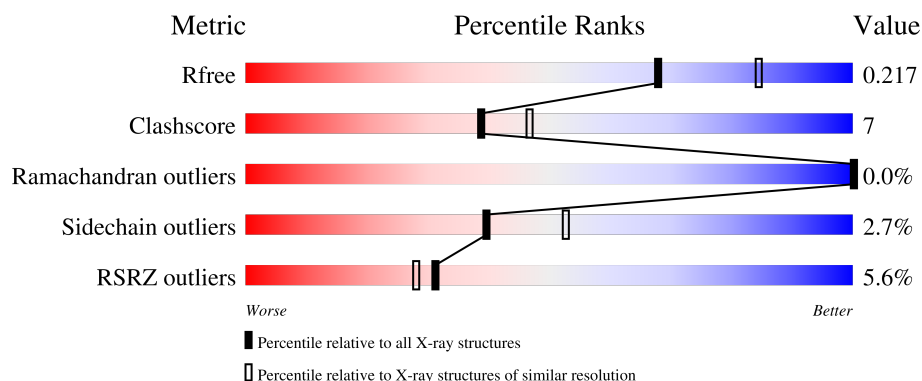
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (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  $\geq 3$ , 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	317	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>• •</div> </div> </div>
1	B	317	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>• •</div> </div> </div>
1	C	317	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>• •</div> </div> </div>
1	D	317	<div> <div>9%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>• •</div> </div> </div>
1	E	317	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	317	
1	G	317	
1	H	317	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22071 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 Endoglucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2602	1694	443	461	4			
1	B	309	Total	C	N	O	S	0	0	0
			2602	1694	443	461	4			
1	C	309	Total	C	N	O	S	0	0	0
			2602	1694	443	461	4			
1	D	309	Total	C	N	O	S	0	0	0
			2602	1694	443	461	4			
1	E	309	Total	C	N	O	S	0	0	0
			2602	1694	443	461	4			
1	F	309	Total	C	N	O	S	0	0	0
			2602	1694	443	461	4			
1	G	309	Total	C	N	O	S	0	0	0
			2602	1694	443	461	4			
1	H	309	Total	C	N	O	S	0	0	0
			2602	1694	443	461	4			

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Cd	0	0
			3	3		
2	B	2	Total	Cd	0	0
			2	2		
2	C	3	Total	Cd	0	0
			3	3		
2	D	2	Total	Cd	0	0
			2	2		
2	E	3	Total	Cd	0	0
			3	3		
2	F	2	Total	Cd	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	3	Total 3	Cd 3	0	0
2	H	2	Total 2	Cd 2	0	0

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total 6	Ni 6	0	0
3	B	5	Total 5	Ni 5	0	0
3	C	6	Total 6	Ni 6	0	0
3	D	3	Total 3	Ni 3	0	0
3	E	4	Total 4	Ni 4	0	0
3	F	4	Total 4	Ni 4	0	0
3	G	4	Total 4	Ni 4	0	0
3	H	4	Total 4	Ni 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	184	Total 184	O 184	0	0
4	B	177	Total 177	O 177	0	0
4	C	83	Total 83	O 83	0	0
4	D	139	Total 139	O 139	0	0
4	E	140	Total 140	O 140	0	0
4	F	123	Total 123	O 123	0	0
4	G	194	Total 194	O 194	0	0

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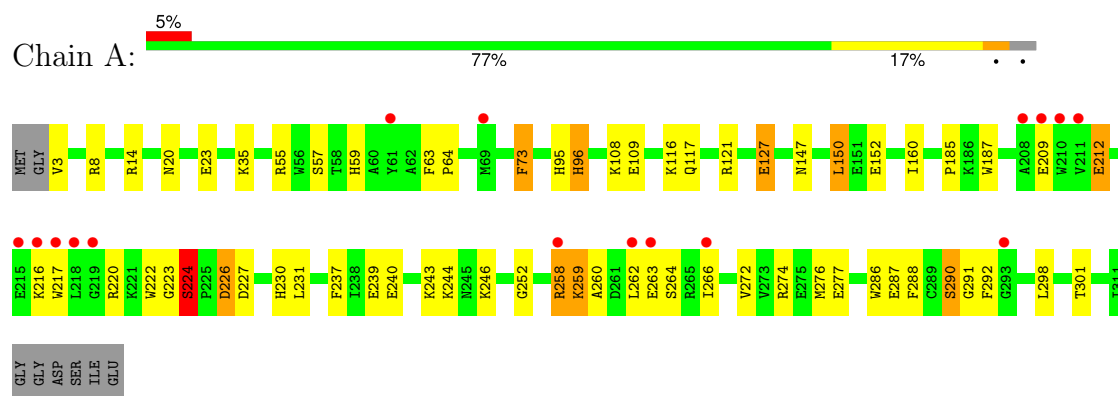
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	159	Total 159	O 159	0	0

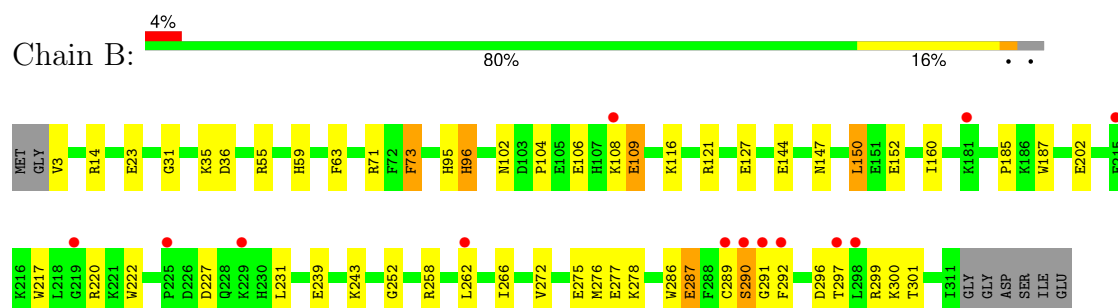
### 3 Residue-property plots [i](#)

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.

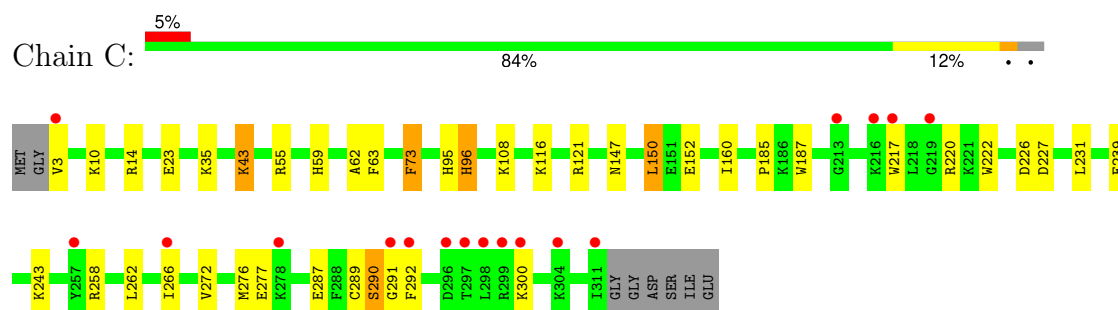
#### • Molecule 1: Endoglucanase



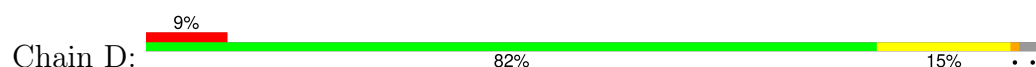
#### • Molecule 1: Endoglucanase

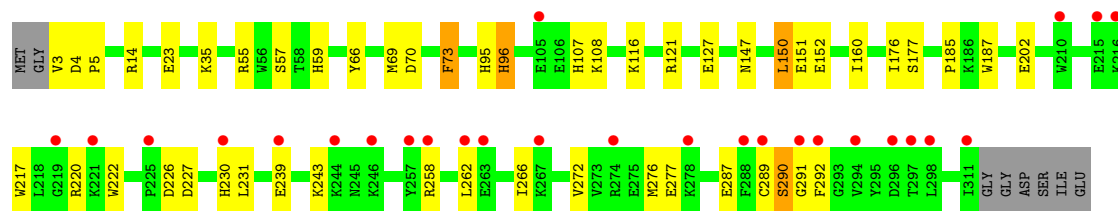


#### • Molecule 1: Endoglucanase

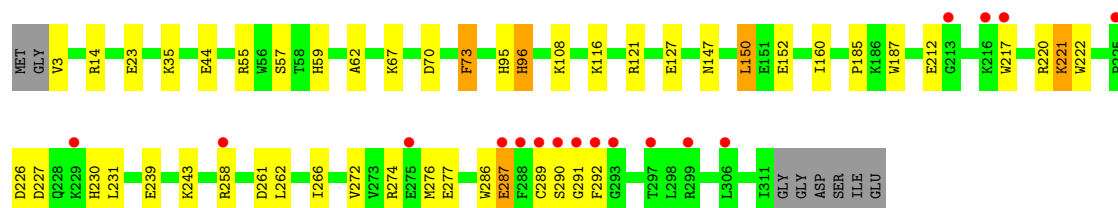
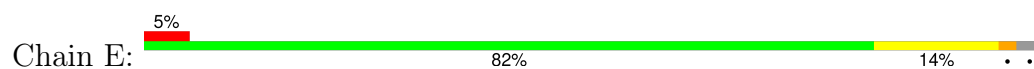


#### • Molecule 1: Endoglucanase

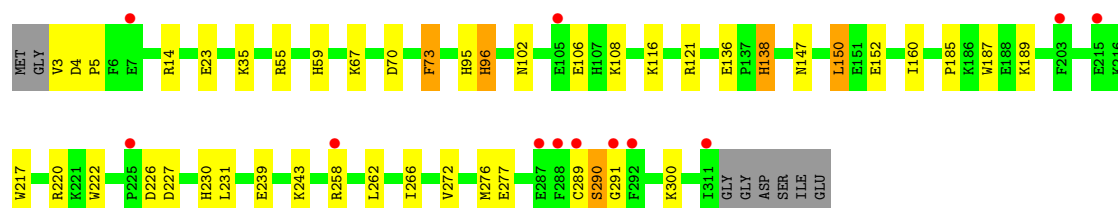
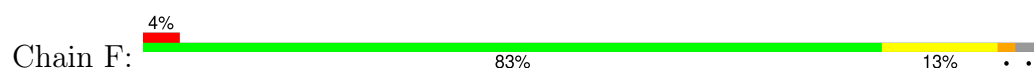




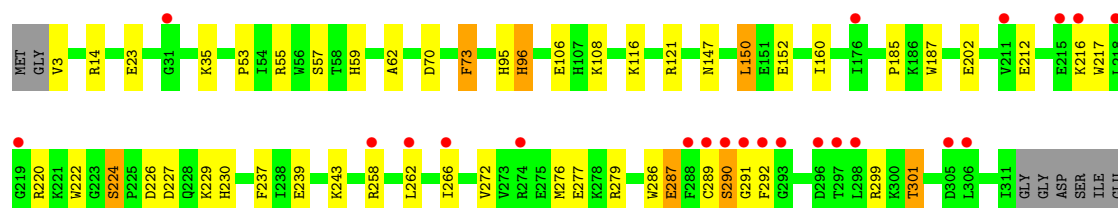
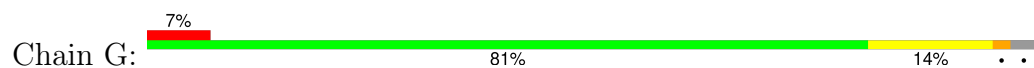
• Molecule 1: Endoglucanase



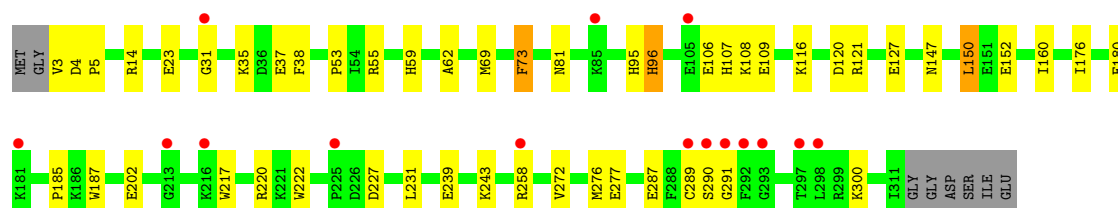
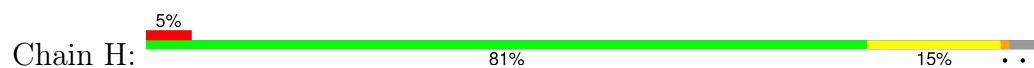
• Molecule 1: Endoglucanase



• Molecule 1: Endoglucanase



• Molecule 1: Endoglucanase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.58Å 95.79Å 103.50Å 64.08° 75.07° 68.73°	Depositor
Resolution (Å)	46.99 – 2.20 46.99 – 2.20	Depositor EDS
% Data completeness (in resolution range)	88.7 (46.99-2.20) 93.9 (46.99-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.205 , 0.218 0.205 , 0.217	Depositor DCC
$R_{free}$ test set	6694 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.7	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 53.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	22071	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CD, NI

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	0.85	8/2683 (0.3%)	0.92	13/3630 (0.4%)
1	B	0.66	4/2683 (0.1%)	0.87	7/3630 (0.2%)
1	C	0.53	3/2683 (0.1%)	0.82	7/3630 (0.2%)
1	D	0.57	6/2683 (0.2%)	0.85	9/3630 (0.2%)
1	E	0.55	4/2683 (0.1%)	0.84	9/3630 (0.2%)
1	F	0.55	5/2683 (0.2%)	0.86	11/3630 (0.3%)
1	G	0.63	5/2683 (0.2%)	0.87	9/3630 (0.2%)
1	H	0.67	5/2683 (0.2%)	0.86	7/3630 (0.2%)
All	All	0.63	40/21464 (0.2%)	0.86	72/29040 (0.2%)

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	GLN	CD-NE2	-6.60	1.19	1.33
1	D	70	ASP	C-O	-5.43	1.17	1.24
1	B	104	PRO	C-O	-5.38	1.17	1.24
1	A	298	LEU	C-O	-5.37	1.17	1.24
1	A	95	HIS	ND1-CE1	5.34	1.37	1.32
1	B	59	HIS	ND1-CE1	5.32	1.37	1.32
1	H	95	HIS	ND1-CE1	5.31	1.37	1.32
1	F	138	HIS	ND1-CE1	5.30	1.37	1.32
1	A	59	HIS	ND1-CE1	5.29	1.37	1.32
1	C	59	HIS	ND1-CE1	5.29	1.37	1.32
1	B	95	HIS	ND1-CE1	5.28	1.37	1.32
1	D	95	HIS	ND1-CE1	5.25	1.37	1.32
1	D	59	HIS	ND1-CE1	5.25	1.37	1.32
1	G	230	HIS	ND1-CE1	5.25	1.37	1.32
1	C	95	HIS	ND1-CE1	5.24	1.37	1.32
1	E	95	HIS	ND1-CE1	5.24	1.37	1.32
1	F	59	HIS	ND1-CE1	5.23	1.37	1.32
1	G	95	HIS	ND1-CE1	5.23	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	106	GLU	C-O	-5.23	1.17	1.24
1	H	59	HIS	ND1-CE1	5.22	1.37	1.32
1	E	59	HIS	ND1-CE1	5.22	1.37	1.32
1	A	230	HIS	ND1-CE1	5.21	1.37	1.32
1	F	95	HIS	ND1-CE1	5.21	1.37	1.32
1	G	59	HIS	ND1-CE1	5.20	1.37	1.32
1	E	230	HIS	ND1-CE1	5.17	1.37	1.32
1	A	301	THR	C-O	-5.16	1.17	1.24
1	F	230	HIS	ND1-CE1	5.14	1.37	1.32
1	A	96	HIS	ND1-CE1	5.12	1.37	1.32
1	C	96	HIS	ND1-CE1	5.12	1.37	1.32
1	D	96	HIS	ND1-CE1	5.11	1.37	1.32
1	F	96	HIS	ND1-CE1	5.11	1.37	1.32
1	G	96	HIS	ND1-CE1	5.09	1.37	1.32
1	B	96	HIS	ND1-CE1	5.09	1.37	1.32
1	E	96	HIS	ND1-CE1	5.08	1.37	1.32
1	D	230	HIS	ND1-CE1	5.06	1.37	1.32
1	A	20	ASN	CG-OD1	5.05	1.33	1.23
1	H	96	HIS	ND1-CE1	5.03	1.37	1.32
1	D	230	HIS	CD2-NE2	-5.03	1.32	1.37
1	H	81	ASN	C-O	-5.01	1.18	1.24
1	G	70	ASP	C-O	-5.01	1.18	1.24

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	ASP	N-CA-C	-7.28	103.43	111.36
1	C	95	HIS	CB-CG-CD2	-6.81	122.34	131.20
1	G	95	HIS	CB-CG-CD2	-6.81	122.34	131.20
1	F	95	HIS	CB-CG-CD2	-6.81	122.35	131.20
1	D	95	HIS	CB-CG-CD2	-6.79	122.37	131.20
1	A	95	HIS	CB-CG-CD2	-6.78	122.39	131.20
1	B	95	HIS	CB-CG-CD2	-6.78	122.39	131.20
1	H	95	HIS	CB-CG-CD2	-6.78	122.39	131.20
1	E	95	HIS	CB-CG-CD2	-6.75	122.42	131.20
1	F	230	HIS	CB-CG-CD2	-6.59	122.63	131.20
1	A	230	HIS	CB-CG-CD2	-6.58	122.65	131.20
1	G	230	HIS	CB-CG-CD2	-6.58	122.65	131.20
1	E	230	HIS	CB-CG-CD2	-6.56	122.67	131.20
1	F	138	HIS	CB-CG-CD2	-6.55	122.68	131.20
1	A	59	HIS	CB-CG-CD2	-6.52	122.73	131.20
1	F	59	HIS	CB-CG-CD2	-6.51	122.73	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	59	HIS	CB-CG-CD2	-6.51	122.73	131.20
1	B	59	HIS	CB-CG-CD2	-6.50	122.75	131.20
1	E	59	HIS	CB-CG-CD2	-6.50	122.76	131.20
1	H	59	HIS	CB-CG-CD2	-6.49	122.76	131.20
1	H	96	HIS	CB-CG-CD2	-6.49	122.76	131.20
1	G	59	HIS	CB-CG-CD2	-6.49	122.77	131.20
1	B	96	HIS	CB-CG-CD2	-6.47	122.79	131.20
1	G	96	HIS	CB-CG-CD2	-6.47	122.80	131.20
1	D	96	HIS	CB-CG-CD2	-6.46	122.80	131.20
1	C	59	HIS	CB-CG-CD2	-6.46	122.81	131.20
1	A	96	HIS	CB-CG-CD2	-6.45	122.81	131.20
1	F	96	HIS	CB-CG-CD2	-6.44	122.82	131.20
1	C	96	HIS	CB-CG-CD2	-6.44	122.83	131.20
1	E	96	HIS	CB-CG-CD2	-6.43	122.84	131.20
1	D	230	HIS	CB-CG-CD2	-6.38	122.91	131.20
1	A	259	LYS	N-CA-C	-6.09	105.11	112.54
1	F	95	HIS	CB-CG-ND1	5.86	131.49	122.70
1	C	95	HIS	CB-CG-ND1	5.85	131.47	122.70
1	H	95	HIS	CB-CG-ND1	5.82	131.43	122.70
1	B	95	HIS	CB-CG-ND1	5.81	131.42	122.70
1	G	95	HIS	CB-CG-ND1	5.81	131.42	122.70
1	A	95	HIS	CB-CG-ND1	5.81	131.41	122.70
1	D	95	HIS	CB-CG-ND1	5.80	131.41	122.70
1	A	258	ARG	O-C-N	5.79	128.26	122.12
1	E	95	HIS	CB-CG-ND1	5.79	131.38	122.70
1	F	138	HIS	CB-CG-ND1	5.71	131.26	122.70
1	F	230	HIS	CB-CG-ND1	5.63	131.15	122.70
1	F	59	HIS	CB-CG-ND1	5.62	131.14	122.70
1	E	59	HIS	CB-CG-ND1	5.62	131.14	122.70
1	H	59	HIS	CB-CG-ND1	5.61	131.11	122.70
1	A	230	HIS	CB-CG-ND1	5.60	131.10	122.70
1	B	59	HIS	CB-CG-ND1	5.60	131.10	122.70
1	E	230	HIS	CB-CG-ND1	5.60	131.10	122.70
1	D	59	HIS	CB-CG-ND1	5.59	131.09	122.70
1	G	230	HIS	CB-CG-ND1	5.58	131.08	122.70
1	A	59	HIS	CB-CG-ND1	5.58	131.07	122.70
1	C	59	HIS	CB-CG-ND1	5.58	131.07	122.70
1	G	59	HIS	CB-CG-ND1	5.58	131.07	122.70
1	B	96	HIS	CB-CG-ND1	5.49	130.94	122.70
1	E	96	HIS	CB-CG-ND1	5.49	130.94	122.70
1	H	96	HIS	CB-CG-ND1	5.49	130.93	122.70
1	G	96	HIS	CB-CG-ND1	5.48	130.92	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	96	HIS	CB-CG-ND1	5.47	130.91	122.70
1	A	96	HIS	CB-CG-ND1	5.45	130.87	122.70
1	D	230	HIS	CB-CG-ND1	5.45	130.87	122.70
1	F	96	HIS	CB-CG-ND1	5.43	130.85	122.70
1	C	96	HIS	CB-CG-ND1	5.42	130.83	122.70
1	A	264	SER	N-CA-C	-5.21	105.72	111.71
1	A	288	PHE	N-CA-C	5.08	116.51	110.97
1	G	289	CYS	N-CA-C	5.05	118.64	112.03
1	D	289	CYS	N-CA-C	5.03	118.62	112.03
1	F	289	CYS	N-CA-C	5.03	118.62	112.03
1	B	289	CYS	N-CA-C	5.02	118.60	112.03
1	E	289	CYS	N-CA-C	5.01	118.60	112.03
1	C	289	CYS	N-CA-C	5.01	118.59	112.03
1	H	289	CYS	N-CA-C	5.00	118.59	112.03

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	2602	0	2537	72	0
1	B	2602	0	2537	44	0
1	C	2602	0	2537	24	0
1	D	2602	0	2537	28	0
1	E	2602	0	2537	30	0
1	F	2602	0	2537	24	0
1	G	2602	0	2537	55	0
1	H	2602	0	2537	39	1
2	A	3	0	0	0	0
2	B	2	0	0	0	0
2	C	3	0	0	0	0
2	D	2	0	0	0	0
2	E	3	0	0	0	0
2	F	2	0	0	0	0
2	G	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	2	0	0	0	0
3	A	6	0	0	1	0
3	B	5	0	0	0	1
3	C	6	0	0	0	0
3	D	3	0	0	0	0
3	E	4	0	0	0	0
3	F	4	0	0	0	0
3	G	4	0	0	0	0
3	H	4	0	0	0	0
4	A	184	0	0	6	0
4	B	177	0	0	9	0
4	C	83	0	0	4	0
4	D	139	0	0	3	0
4	E	140	0	0	4	0
4	F	123	0	0	2	0
4	G	194	0	0	10	0
4	H	159	0	0	9	0
All	All	22071	0	20296	275	1

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 7.

All (275) 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:E:127:GLU:HG3	4:E:833:HOH:O	1.39	1.20
1:C:300:LYS:HD2	4:C:366:HOH:O	1.37	1.16
1:A:244:LYS:NZ	1:H:300:LYS:HD2	1.68	1.09
4:E:1297:HOH:O	1:F:102:ASN:HB3	1.55	1.05
1:A:8:ARG:NH2	1:A:127:GLU:HG2	1.72	1.03
1:A:244:LYS:CE	1:H:300:LYS:HD2	1.89	1.03
1:A:244:LYS:HZ1	1:H:300:LYS:HD2	1.22	1.01
1:B:127:GLU:HG3	4:B:391:HOH:O	1.61	0.99
1:A:216:LYS:NZ	1:G:237:PHE:CD1	2.30	0.99
1:G:216:LYS:HD2	4:G:343:HOH:O	1.63	0.98
1:A:244:LYS:HZ1	1:H:300:LYS:CD	1.76	0.97
1:A:237:PHE:CD1	1:G:216:LYS:NZ	2.33	0.96
1:A:237:PHE:CE1	1:G:216:LYS:NZ	2.33	0.96
4:C:1373:HOH:O	1:D:57:SER:HB2	1.67	0.95
1:E:286:TRP:CD1	1:E:287:GLU:HG3	2.01	0.94
1:G:287:GLU:OE2	1:G:292:PHE:HB2	1.71	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:287:GLU:OE2	1:E:292:PHE:HB2	1.71	0.90
1:A:244:LYS:HE3	1:H:300:LYS:HD2	1.52	0.89
1:D:152:GLU:HG2	4:D:1380:HOH:O	1.72	0.87
1:H:127:GLU:HG3	4:H:362:HOH:O	1.73	0.86
1:C:287:GLU:OE2	1:C:292:PHE:HB2	1.77	0.85
1:A:209:GLU:HG2	1:B:258:ARG:HH22	1.39	0.85
1:D:127:GLU:HG3	4:D:1329:HOH:O	1.76	0.84
1:A:216:LYS:NZ	1:G:237:PHE:HD1	1.72	0.83
1:A:287:GLU:OE1	1:A:292:PHE:HB2	1.79	0.83
1:A:216:LYS:NZ	1:G:237:PHE:CE1	2.49	0.80
1:B:102:ASN:HB3	4:B:1237:HOH:O	1.81	0.79
1:A:226:ASP:OD2	3:A:322:NI:NI	1.29	0.77
1:A:262:LEU:O	1:A:266:ILE:HG12	1.84	0.76
1:B:109:GLU:HG3	4:B:537:HOH:O	1.86	0.76
1:E:286:TRP:CE2	1:E:287:GLU:HG2	2.20	0.76
1:A:244:LYS:HZ1	1:H:300:LYS:CE	1.99	0.76
1:H:109:GLU:HG3	4:H:355:HOH:O	1.87	0.73
1:A:237:PHE:HD1	1:G:216:LYS:NZ	1.87	0.73
1:E:286:TRP:CG	1:E:287:GLU:HG3	2.23	0.72
1:A:246:LYS:NZ	4:A:364:HOH:O	2.22	0.72
1:A:237:PHE:HE1	1:G:216:LYS:NZ	1.87	0.72
1:D:287:GLU:OE2	1:D:292:PHE:N	2.23	0.72
1:G:229:LYS:NZ	4:G:1391:HOH:O	2.23	0.70
1:A:258:ARG:NH2	1:A:291:GLY:HA2	2.08	0.69
1:H:258:ARG:NH2	1:H:291:GLY:HA2	2.09	0.68
1:A:244:LYS:HE3	1:H:300:LYS:CD	2.23	0.68
1:G:258:ARG:NH2	1:G:291:GLY:HA2	2.09	0.68
1:D:258:ARG:NH2	1:D:291:GLY:HA2	2.09	0.68
1:H:37:GLU:HB2	4:H:1326:HOH:O	1.92	0.68
1:E:258:ARG:NH2	1:E:291:GLY:HA2	2.09	0.68
1:A:147:ASN:HA	1:A:150:LEU:HD13	1.76	0.68
1:C:258:ARG:NH2	1:C:291:GLY:HA2	2.09	0.68
1:F:147:ASN:HA	1:F:150:LEU:HD13	1.76	0.68
1:B:147:ASN:HA	1:B:150:LEU:HD13	1.76	0.67
1:F:258:ARG:NH2	1:F:291:GLY:HA2	2.09	0.67
1:G:147:ASN:HA	1:G:150:LEU:HD13	1.76	0.67
1:C:147:ASN:HA	1:C:150:LEU:HD13	1.76	0.66
1:D:147:ASN:HA	1:D:150:LEU:HD13	1.76	0.66
1:H:147:ASN:HA	1:H:150:LEU:HD13	1.76	0.66
1:E:147:ASN:HA	1:E:150:LEU:HD13	1.76	0.65
1:A:220:ARG:NH1	4:A:1392:HOH:O	2.23	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LYS:CE	1:G:237:PHE:CD1	2.79	0.64
1:E:116:LYS:HE3	4:E:1069:HOH:O	1.97	0.64
1:B:286:TRP:C	1:B:287:GLU:HG3	2.17	0.63
1:A:237:PHE:CD1	1:G:216:LYS:CE	2.81	0.63
1:C:272:VAL:HG12	1:C:276:MET:HE2	1.81	0.63
1:D:272:VAL:HG12	1:D:276:MET:HE2	1.81	0.63
1:H:272:VAL:HG12	1:H:276:MET:HE2	1.81	0.63
1:E:272:VAL:HG12	1:E:276:MET:HE2	1.81	0.62
1:A:272:VAL:HG12	1:A:276:MET:HE2	1.81	0.62
1:G:272:VAL:HG12	1:G:276:MET:HE2	1.81	0.61
1:B:272:VAL:HG12	1:B:276:MET:HE2	1.81	0.61
1:F:272:VAL:HG12	1:F:276:MET:HE2	1.81	0.60
1:G:202:GLU:HG3	4:G:1058:HOH:O	2.01	0.60
1:A:237:PHE:CE1	1:G:216:LYS:CE	2.83	0.60
1:E:286:TRP:CD1	1:E:287:GLU:CG	2.82	0.60
1:B:202:GLU:HG3	4:B:1032:HOH:O	2.02	0.59
1:B:286:TRP:CD1	1:B:287:GLU:HG2	2.38	0.59
1:D:151:GLU:HG3	1:D:185:PRO:HG2	1.85	0.58
1:G:216:LYS:CD	4:G:343:HOH:O	2.35	0.58
1:G:229:LYS:CE	4:G:1391:HOH:O	2.51	0.58
1:B:296:ASP:C	1:B:296:ASP:OD1	2.46	0.57
1:G:212:GLU:HG3	1:H:31:GLY:O	2.05	0.57
1:E:286:TRP:CE2	1:E:287:GLU:CG	2.86	0.57
1:E:57:SER:HB2	4:F:1181:HOH:O	2.04	0.56
1:H:202:GLU:HG3	4:H:785:HOH:O	2.05	0.56
1:C:116:LYS:HG3	1:C:160:ILE:HD11	1.88	0.56
1:H:35:LYS:HG3	1:H:38:PHE:CZ	2.41	0.56
1:G:299:ARG:C	1:G:301:THR:HG22	2.31	0.56
1:G:116:LYS:HG3	1:G:160:ILE:HD11	1.88	0.55
1:H:116:LYS:HG3	1:H:160:ILE:HD11	1.88	0.55
1:G:224:SER:O	1:G:227:ASP:HB2	2.06	0.55
1:A:116:LYS:HG3	1:A:160:ILE:HD11	1.88	0.55
1:A:237:PHE:CE1	1:G:216:LYS:HE3	2.41	0.55
1:E:116:LYS:HG3	1:E:160:ILE:HD11	1.88	0.55
1:D:116:LYS:HG3	1:D:160:ILE:HD11	1.88	0.55
1:F:136:GLU:O	1:F:138:HIS:HD2	1.90	0.55
1:A:216:LYS:CE	1:G:237:PHE:HD1	2.16	0.54
1:E:62:ALA:N	1:F:106:GLU:OE1	2.28	0.54
1:B:116:LYS:HG3	1:B:160:ILE:HD11	1.88	0.54
1:F:116:LYS:HG3	1:F:160:ILE:HD11	1.88	0.54
1:E:286:TRP:NE1	1:E:287:GLU:CG	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:221:LYS:HG3	1:E:261:ASP:OD1	2.08	0.53
1:G:286:TRP:CD1	1:G:287:GLU:HG3	2.44	0.53
1:G:57:SER:HB2	4:H:653:HOH:O	2.08	0.52
1:A:212:GLU:HG3	1:B:31:GLY:O	2.10	0.52
1:G:229:LYS:HE2	4:G:1391:HOH:O	2.08	0.52
1:F:67:LYS:NZ	1:F:70:ASP:OD1	2.43	0.52
1:A:244:LYS:CE	1:H:300:LYS:CD	2.77	0.52
1:D:14:ARG:HD3	1:D:277:GLU:OE2	2.11	0.51
1:G:239:GLU:CD	1:G:279:ARG:HG2	2.36	0.51
1:B:14:ARG:HD3	1:B:277:GLU:OE2	2.11	0.51
1:H:14:ARG:HD3	1:H:277:GLU:OE2	2.11	0.51
1:E:23:GLU:HA	1:E:55:ARG:HB2	1.93	0.51
1:A:23:GLU:HA	1:A:55:ARG:HB2	1.93	0.50
1:H:23:GLU:HA	1:H:55:ARG:HB2	1.93	0.50
1:G:14:ARG:HD3	1:G:277:GLU:OE2	2.11	0.50
1:A:63:PHE:CE1	1:B:63:PHE:HD1	2.28	0.50
1:A:223:GLY:O	1:A:224:SER:O	2.30	0.50
1:C:14:ARG:HD3	1:C:277:GLU:OE2	2.11	0.50
1:D:23:GLU:HA	1:D:55:ARG:HB2	1.93	0.50
1:G:286:TRP:CG	1:G:287:GLU:HG3	2.47	0.50
4:C:888:HOH:O	1:F:300:LYS:HG3	2.12	0.50
1:A:14:ARG:HD3	1:A:277:GLU:OE2	2.11	0.50
1:E:14:ARG:HD3	1:E:277:GLU:OE2	2.11	0.50
1:B:55:ARG:HD2	1:B:96:HIS:HB2	1.94	0.49
1:F:14:ARG:HD3	1:F:277:GLU:OE2	2.11	0.49
1:G:55:ARG:HD2	1:G:96:HIS:HB2	1.94	0.49
1:G:286:TRP:C	1:G:287:GLU:HG3	2.37	0.49
1:A:217:TRP:O	1:A:220:ARG:HB2	2.13	0.49
1:F:23:GLU:HA	1:F:55:ARG:HB2	1.93	0.49
1:B:23:GLU:HA	1:B:55:ARG:HB2	1.93	0.49
1:C:23:GLU:HA	1:C:55:ARG:HB2	1.93	0.49
1:A:223:GLY:C	1:A:224:SER:O	2.54	0.49
1:C:55:ARG:HD2	1:C:96:HIS:HB2	1.94	0.49
1:B:296:ASP:OD2	1:B:299:ARG:NH1	2.46	0.49
1:D:217:TRP:O	1:D:220:ARG:HB2	2.13	0.49
1:G:217:TRP:O	1:G:220:ARG:HB2	2.13	0.49
1:C:217:TRP:O	1:C:220:ARG:HB2	2.12	0.49
1:H:55:ARG:HD2	1:H:96:HIS:HB2	1.95	0.49
1:H:217:TRP:O	1:H:220:ARG:HB2	2.12	0.49
1:B:297:THR:O	1:B:300:LYS:HG2	2.13	0.49
1:F:55:ARG:HD2	1:F:96:HIS:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:23:GLU:HA	1:G:55:ARG:HB2	1.93	0.49
1:B:217:TRP:O	1:B:220:ARG:HB2	2.13	0.49
1:E:55:ARG:HD2	1:E:96:HIS:HB2	1.94	0.48
1:A:63:PHE:CD1	1:B:63:PHE:CD1	3.02	0.48
1:E:217:TRP:O	1:E:220:ARG:HB2	2.12	0.48
1:A:63:PHE:CE1	1:B:63:PHE:CD1	3.02	0.48
1:B:296:ASP:O	1:B:300:LYS:N	2.46	0.48
1:A:55:ARG:HD2	1:A:96:HIS:HB2	1.94	0.48
1:A:55:ARG:NH2	4:A:1368:HOH:O	2.43	0.48
1:D:55:ARG:HD2	1:D:96:HIS:HB2	1.94	0.48
1:G:55:ARG:NH2	4:G:1362:HOH:O	2.44	0.48
1:B:275:GLU:OE2	1:B:278:LYS:HE2	2.13	0.48
1:F:217:TRP:O	1:F:220:ARG:HB2	2.12	0.48
1:D:185:PRO:HB3	1:D:187:TRP:NE1	2.29	0.48
1:C:43:LYS:HD2	1:C:43:LYS:HA	1.55	0.47
1:C:185:PRO:HB3	1:C:187:TRP:NE1	2.29	0.47
1:E:185:PRO:HB3	1:E:187:TRP:NE1	2.29	0.47
1:H:185:PRO:HB3	1:H:187:TRP:NE1	2.29	0.47
1:A:109:GLU:OE1	1:D:66:TYR:HE2	1.97	0.47
1:G:185:PRO:HB3	1:G:187:TRP:NE1	2.29	0.47
1:B:71:ARG:NH1	4:B:1239:HOH:O	2.46	0.47
1:D:202:GLU:OE1	4:D:419:HOH:O	2.21	0.47
1:B:185:PRO:HB3	1:B:187:TRP:NE1	2.29	0.47
1:B:287:GLU:OE2	1:B:292:PHE:HB2	2.15	0.47
1:F:185:PRO:HB3	1:F:187:TRP:NE1	2.29	0.47
1:G:62:ALA:HB2	1:H:107:HIS:NE2	2.30	0.47
1:B:258:ARG:NH1	1:B:291:GLY:HA2	2.29	0.46
1:G:212:GLU:HB2	4:H:383:HOH:O	2.16	0.46
1:A:185:PRO:HB3	1:A:187:TRP:NE1	2.29	0.46
1:A:57:SER:HB2	4:B:355:HOH:O	2.15	0.46
1:A:209:GLU:HG2	1:B:258:ARG:NH2	2.18	0.46
1:C:290:SER:HB3	1:C:291:GLY:H	1.57	0.46
1:B:252:GLY:HA3	4:B:325:HOH:O	2.16	0.45
1:C:287:GLU:OE2	1:C:292:PHE:CB	2.58	0.45
1:H:120:ASP:OD1	4:H:364:HOH:O	2.21	0.45
1:A:216:LYS:HE3	1:G:237:PHE:CE1	2.51	0.45
1:G:73:PHE:CD1	1:G:121:ARG:HD3	2.51	0.45
1:C:73:PHE:CD1	1:C:121:ARG:HD3	2.51	0.45
1:A:73:PHE:CD1	1:A:121:ARG:HD3	2.51	0.45
1:A:239:GLU:HG2	1:A:243:LYS:HE3	1.98	0.45
1:G:108:LYS:HD2	1:G:152:GLU:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:73:PHE:CD1	1:E:121:ARG:HD3	2.51	0.45
1:H:73:PHE:CD1	1:H:121:ARG:HD3	2.51	0.45
1:A:222:TRP:CE2	1:A:227:ASP:HB3	2.52	0.45
1:B:73:PHE:CD1	1:B:121:ARG:HD3	2.52	0.45
1:C:35:LYS:HA	1:C:35:LYS:HD3	1.79	0.45
1:E:108:LYS:HD2	1:E:152:GLU:OE1	2.17	0.45
1:H:37:GLU:CB	4:H:1326:HOH:O	2.58	0.45
1:C:108:LYS:HD2	1:C:152:GLU:OE1	2.17	0.45
1:G:220:ARG:NH1	4:G:1233:HOH:O	2.34	0.45
1:D:73:PHE:CD1	1:D:121:ARG:HD3	2.51	0.45
1:F:108:LYS:HD2	1:F:152:GLU:OE1	2.17	0.45
1:A:35:LYS:HA	1:A:35:LYS:HD3	1.79	0.44
1:F:73:PHE:CD1	1:F:121:ARG:HD3	2.51	0.44
1:A:108:LYS:HD2	1:A:152:GLU:OE1	2.17	0.44
1:A:216:LYS:CE	1:G:237:PHE:CE1	2.98	0.44
1:F:4:ASP:HA	1:F:5:PRO:HD2	1.90	0.44
1:A:63:PHE:HD1	1:B:63:PHE:CE1	2.36	0.44
1:A:287:GLU:OE1	1:A:287:GLU:N	2.50	0.44
1:B:108:LYS:HD2	1:B:152:GLU:OE1	2.17	0.44
1:D:108:LYS:HD2	1:D:152:GLU:OE1	2.17	0.44
1:H:108:LYS:HD2	1:H:152:GLU:OE1	2.17	0.44
1:A:259:LYS:O	4:A:997:HOH:O	2.21	0.44
1:B:286:TRP:CE2	1:B:287:GLU:HG2	2.53	0.44
1:E:274:ARG:HD2	4:E:397:HOH:O	2.17	0.44
1:F:35:LYS:HA	1:F:35:LYS:HD3	1.79	0.44
1:D:290:SER:HB3	1:D:291:GLY:H	1.57	0.44
1:B:299:ARG:O	1:B:300:LYS:C	2.59	0.43
1:A:237:PHE:HD1	1:G:216:LYS:CE	2.26	0.43
1:C:55:ARG:NH2	4:C:1371:HOH:O	2.42	0.43
1:A:8:ARG:HH22	1:A:127:GLU:HG2	1.74	0.43
1:A:274:ARG:NH1	4:A:839:HOH:O	2.51	0.43
1:B:35:LYS:HA	1:B:35:LYS:HD3	1.79	0.43
4:G:1358:HOH:O	1:H:69:MET:HE1	2.19	0.43
1:A:63:PHE:CD1	1:B:63:PHE:CE1	3.07	0.42
1:A:290:SER:HB3	1:A:291:GLY:H	1.59	0.42
1:A:244:LYS:NZ	1:H:300:LYS:CD	2.47	0.42
1:B:286:TRP:CG	1:B:287:GLU:HG2	2.54	0.42
1:D:4:ASP:HA	1:D:5:PRO:HD2	1.90	0.42
1:G:35:LYS:HA	1:G:35:LYS:HD3	1.79	0.42
1:A:286:TRP:HA	1:A:287:GLU:HA	1.81	0.42
1:A:216:LYS:HE3	1:G:237:PHE:CD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:ARG:C	1:A:260:ALA:N	2.74	0.42
1:F:189:LYS:HG3	4:F:1035:HOH:O	2.19	0.42
1:B:36:ASP:OD2	4:B:454:HOH:O	2.22	0.42
1:E:239:GLU:HG2	1:E:243:LYS:HE3	2.02	0.42
1:F:290:SER:HB3	1:F:291:GLY:H	1.57	0.41
1:G:239:GLU:HG2	1:G:243:LYS:HE3	2.02	0.41
1:A:231:LEU:HD11	1:A:272:VAL:HG22	2.03	0.41
1:A:252:GLY:HA3	4:A:361:HOH:O	2.20	0.41
1:C:62:ALA:HB2	1:D:107:HIS:NE2	2.35	0.41
1:D:222:TRP:CE2	1:D:227:ASP:HB3	2.56	0.41
1:G:290:SER:HB3	1:G:291:GLY:H	1.57	0.41
1:A:64:PRO:HG2	1:C:63:PHE:CZ	2.55	0.41
1:A:209:GLU:OE2	1:A:259:LYS:HE3	2.20	0.41
1:G:222:TRP:CE2	1:G:227:ASP:HB3	2.56	0.41
1:A:222:TRP:CE3	1:A:223:GLY:HA2	2.55	0.41
1:D:35:LYS:HD3	1:D:35:LYS:HA	1.79	0.41
1:E:222:TRP:CE2	1:E:227:ASP:HB3	2.56	0.41
1:E:231:LEU:HD11	1:E:272:VAL:HG22	2.02	0.41
1:F:231:LEU:HD11	1:F:272:VAL:HG22	2.03	0.41
1:B:231:LEU:HD11	1:B:272:VAL:HG22	2.02	0.41
1:H:152:GLU:HG2	4:H:428:HOH:O	2.21	0.41
1:A:152:GLU:OE2	1:D:116:LYS:NZ	2.54	0.41
1:E:35:LYS:HA	1:E:35:LYS:HD3	1.79	0.41
1:F:222:TRP:CE2	1:F:227:ASP:HB3	2.56	0.41
1:H:239:GLU:HG2	1:H:243:LYS:HE3	2.02	0.41
1:B:222:TRP:CE2	1:B:227:ASP:HB3	2.56	0.41
1:C:222:TRP:CE2	1:C:227:ASP:HB3	2.56	0.41
1:C:262:LEU:O	1:C:266:ILE:HG12	2.21	0.41
1:G:262:LEU:O	1:G:266:ILE:HG12	2.21	0.41
1:H:222:TRP:CE2	1:H:227:ASP:HB3	2.56	0.41
1:H:231:LEU:HD11	1:H:272:VAL:HG22	2.03	0.41
1:B:262:LEU:O	1:B:266:ILE:HG12	2.21	0.41
1:C:231:LEU:HD11	1:C:272:VAL:HG22	2.03	0.41
1:D:231:LEU:HD11	1:D:272:VAL:HG22	2.03	0.41
1:D:262:LEU:O	1:D:266:ILE:HG12	2.21	0.41
1:G:286:TRP:CE2	1:G:287:GLU:HG2	2.56	0.41
1:G:299:ARG:CB	1:G:301:THR:CG2	2.98	0.41
1:E:67:LYS:NZ	1:E:70:ASP:OD1	2.51	0.41
1:E:262:LEU:O	1:E:266:ILE:HG12	2.21	0.41
1:A:226:ASP:O	1:A:227:ASP:C	2.63	0.40
1:B:290:SER:HB3	1:B:291:GLY:H	1.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:GLU:HG3	1:D:185:PRO:CG	2.49	0.40
1:C:239:GLU:HG2	1:C:243:LYS:HE3	2.02	0.40
1:G:106:GLU:OE1	1:H:62:ALA:N	2.35	0.40
1:H:23:GLU:HB3	1:H:53:PRO:HB2	2.04	0.40
1:B:239:GLU:HG2	1:B:243:LYS:HE3	2.02	0.40
1:D:239:GLU:HG2	1:D:243:LYS:HE3	2.02	0.40
1:F:239:GLU:HG2	1:F:243:LYS:HE3	2.02	0.40
1:B:144:GLU:HG3	4:B:664:HOH:O	2.21	0.40
4:G:1358:HOH:O	1:H:69:MET:CE	2.69	0.40
1:H:176:ILE:HD13	1:H:176:ILE:HG21	1.73	0.40
1:F:262:LEU:O	1:F:266:ILE:HG12	2.21	0.40
1:G:23:GLU:HB3	1:G:53:PRO:HB2	2.04	0.40
1:H:4:ASP:HA	1:H:5:PRO:HD2	1.90	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:180:GLU:OE2	3:B:321:NI:NI[1_465]	1.50	0.70

## 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	307/317 (97%)	298 (97%)	8 (3%)	1 (0%)	37	42
1	B	307/317 (97%)	296 (96%)	11 (4%)	0	100	100
1	C	307/317 (97%)	298 (97%)	9 (3%)	0	100	100
1	D	307/317 (97%)	298 (97%)	9 (3%)	0	100	100
1	E	307/317 (97%)	298 (97%)	9 (3%)	0	100	100
1	F	307/317 (97%)	297 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	307/317 (97%)	299 (97%)	8 (3%)	0	100	100
1	H	307/317 (97%)	295 (96%)	12 (4%)	0	100	100
All	All	2456/2536 (97%)	2379 (97%)	76 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	SER

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	272/277 (98%)	263 (97%)	9 (3%)	33	44
1	B	272/277 (98%)	264 (97%)	8 (3%)	37	50
1	C	272/277 (98%)	265 (97%)	7 (3%)	41	54
1	D	272/277 (98%)	264 (97%)	8 (3%)	37	50
1	E	272/277 (98%)	263 (97%)	9 (3%)	33	44
1	F	272/277 (98%)	267 (98%)	5 (2%)	54	69
1	G	272/277 (98%)	264 (97%)	8 (3%)	37	50
1	H	272/277 (98%)	267 (98%)	5 (2%)	54	69
All	All	2176/2216 (98%)	2117 (97%)	59 (3%)	40	53

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	73	PHE
1	A	127	GLU
1	A	150	LEU
1	A	212	GLU
1	A	224	SER

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Mol	Chain	Res	Type
1	A	240	GLU
1	A	263	GLU
1	A	290	SER
1	B	3	VAL
1	B	73	PHE
1	B	106	GLU
1	B	109	GLU
1	B	150	LEU
1	B	287	GLU
1	B	290	SER
1	B	301	THR
1	C	3	VAL
1	C	10	LYS
1	C	43	LYS
1	C	73	PHE
1	C	150	LEU
1	C	226	ASP
1	C	290	SER
1	D	3	VAL
1	D	69	MET
1	D	73	PHE
1	D	150	LEU
1	D	176	ILE
1	D	177	SER
1	D	226	ASP
1	D	290	SER
1	E	3	VAL
1	E	44	GLU
1	E	73	PHE
1	E	150	LEU
1	E	212	GLU
1	E	221	LYS
1	E	226	ASP
1	E	287	GLU
1	E	290	SER
1	F	3	VAL
1	F	73	PHE
1	F	150	LEU
1	F	226	ASP
1	F	290	SER
1	G	3	VAL
1	G	73	PHE

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Mol	Chain	Res	Type
1	G	150	LEU
1	G	224	SER
1	G	226	ASP
1	G	287	GLU
1	G	290	SER
1	G	301	THR
1	H	3	VAL
1	H	73	PHE
1	H	150	LEU
1	H	287	GLU
1	H	290	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	20	ASN
1	B	81	ASN
1	E	81	ASN
1	F	81	ASN
1	F	138	HIS
1	G	81	ASN
1	H	20	ASN

### 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 [i](#)

Of 56 ligands modelled in this entry, 56 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 [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	309/317 (97%)	0.35	16 (5%) 34 30	21, 38, 66, 121	0
1	B	309/317 (97%)	0.37	13 (4%) 41 37	23, 42, 73, 88	0
1	C	309/317 (97%)	0.56	17 (5%) 32 28	28, 54, 92, 146	0
1	D	309/317 (97%)	0.58	27 (8%) 17 15	22, 49, 99, 131	0
1	E	309/317 (97%)	0.45	17 (5%) 32 28	25, 44, 90, 112	0
1	F	309/317 (97%)	0.53	12 (3%) 44 40	24, 51, 101, 118	0
1	G	309/317 (97%)	0.38	22 (7%) 23 21	23, 41, 77, 114	0
1	H	309/317 (97%)	0.39	15 (4%) 36 33	23, 41, 70, 95	0
All	All	2472/2536 (97%)	0.45	139 (5%) 31 28	21, 44, 87, 146	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	289	CYS	5.6
1	G	216	LYS	5.0
1	F	289	CYS	4.9
1	E	292	PHE	4.8
1	D	219	GLY	4.7
1	A	216	LYS	4.6
1	E	291	GLY	4.4
1	G	289	CYS	4.1
1	C	213	GLY	4.0
1	F	292	PHE	4.0
1	E	288	PHE	3.9
1	D	298	LEU	3.9
1	B	289	CYS	3.8
1	C	219	GLY	3.8
1	C	298	LEU	3.7
1	B	291	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	291	GLY	3.7
1	G	291	GLY	3.6
1	G	297	THR	3.6
1	G	298	LEU	3.6
1	A	266	ILE	3.5
1	G	290	SER	3.4
1	G	292	PHE	3.4
1	C	311	ILE	3.3
1	E	293	GLY	3.3
1	H	297	THR	3.2
1	D	297	THR	3.2
1	F	311	ILE	3.2
1	C	299	ARG	3.1
1	D	257	TYR	3.1
1	A	293	GLY	3.1
1	D	262	LEU	3.1
1	H	213	GLY	3.1
1	G	293	GLY	3.0
1	H	298	LEU	3.0
1	A	215	GLU	3.0
1	B	290	SER	3.0
1	F	258	ARG	3.0
1	F	215	GLU	3.0
1	H	289	CYS	3.0
1	F	288	PHE	3.0
1	D	225	PRO	3.0
1	H	105	GLU	2.9
1	D	216	LYS	2.9
1	A	219	GLY	2.9
1	H	258	ARG	2.9
1	A	258	ARG	2.9
1	D	311	ILE	2.9
1	C	216	LYS	2.9
1	H	293	GLY	2.8
1	C	296	ASP	2.8
1	D	215	GLU	2.8
1	A	218	LEU	2.7
1	D	105	GLU	2.7
1	B	225	PRO	2.7
1	D	292	PHE	2.7
1	B	108	LYS	2.7
1	D	289	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	292	PHE	2.7
1	D	258	ARG	2.6
1	F	225	PRO	2.6
1	G	296	ASP	2.6
1	C	3	VAL	2.6
1	G	288	PHE	2.6
1	D	274	ARG	2.5
1	G	258	ARG	2.5
1	C	266	ILE	2.5
1	C	292	PHE	2.5
1	D	288	PHE	2.5
1	H	181	LYS	2.5
1	G	266	ILE	2.5
1	B	297	THR	2.5
1	E	225	PRO	2.5
1	D	263	GLU	2.4
1	D	296	ASP	2.4
1	C	300	LYS	2.4
1	B	181	LYS	2.4
1	H	216	LYS	2.4
1	G	262	LEU	2.4
1	E	275	GLU	2.4
1	D	278	LYS	2.4
1	E	299	ARG	2.4
1	G	219	GLY	2.4
1	D	210	TRP	2.3
1	A	208	ALA	2.3
1	D	294	VAL	2.3
1	C	278	LYS	2.3
1	H	292	PHE	2.3
1	A	262	LEU	2.3
1	G	274	ARG	2.3
1	E	290	SER	2.3
1	B	219	GLY	2.3
1	B	298	LEU	2.3
1	E	287	GLU	2.3
1	C	297	THR	2.3
1	H	291	GLY	2.3
1	B	229	LYS	2.2
1	D	239	GLU	2.2
1	B	262	LEU	2.2
1	E	306	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	287	GLU	2.2
1	G	306	LEU	2.2
1	E	258	ARG	2.2
1	C	304	LYS	2.2
1	A	217	TRP	2.2
1	C	217	TRP	2.2
1	C	291	GLY	2.2
1	D	291	GLY	2.2
1	E	213	GLY	2.2
1	H	31	GLY	2.2
1	F	105	GLU	2.2
1	A	210	TRP	2.2
1	G	218	LEU	2.2
1	E	297	THR	2.2
1	H	290	SER	2.1
1	G	31	GLY	2.1
1	A	211	VAL	2.1
1	G	215	GLU	2.1
1	D	230	HIS	2.1
1	E	229	LYS	2.1
1	H	85	LYS	2.1
1	A	61	TYR	2.1
1	A	209	GLU	2.1
1	B	215	GLU	2.1
1	D	244	LYS	2.1
1	D	246	LYS	2.1
1	D	267	LYS	2.1
1	E	216	LYS	2.1
1	A	263	GLU	2.1
1	G	305	ASP	2.1
1	D	221	LYS	2.1
1	F	7	GLU	2.0
1	C	257	TYR	2.0
1	H	225	PRO	2.0
1	A	69	MET	2.0
1	E	217	TRP	2.0
1	G	211	VAL	2.0
1	F	203	PHE	2.0
1	G	176	ILE	2.0

## 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 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
3	NI	C	325	1/1	0.60	0.17	143,143,143,143	0
3	NI	F	320	1/1	0.68	0.12	135,135,135,135	0
3	NI	E	323	1/1	0.71	0.21	108,108,108,108	0
3	NI	F	321	1/1	0.75	0.18	127,127,127,127	0
3	NI	D	322	1/1	0.77	0.16	109,109,109,109	0
3	NI	C	326	1/1	0.77	0.12	106,106,106,106	0
2	CD	A	319	1/1	0.78	0.13	42,42,42,42	0
3	NI	C	324	1/1	0.81	0.15	115,115,115,115	0
3	NI	B	324	1/1	0.83	0.15	92,92,92,92	0
3	NI	G	322	1/1	0.83	0.10	108,108,108,108	0
3	NI	H	322	1/1	0.83	0.16	86,86,86,86	0
3	NI	E	322	1/1	0.84	0.14	121,121,121,121	0
3	NI	E	324	1/1	0.84	0.12	94,94,94,94	0
3	NI	C	323	1/1	0.85	0.12	98,98,98,98	0
3	NI	A	324	1/1	0.85	0.10	94,94,94,94	0
3	NI	A	325	1/1	0.86	0.10	85,85,85,85	0
3	NI	G	323	1/1	0.86	0.11	95,95,95,95	0
3	NI	G	324	1/1	0.86	0.10	99,99,99,99	0
3	NI	C	322	1/1	0.86	0.11	123,123,123,123	0
3	NI	F	323	1/1	0.87	0.12	105,105,105,105	0
3	NI	F	322	1/1	0.88	0.09	78,78,78,78	0
3	NI	A	326	1/1	0.88	0.11	71,71,71,71	0
3	NI	B	323	1/1	0.88	0.10	76,76,76,76	0
2	CD	C	319	1/1	0.89	0.10	53,53,53,53	0
3	NI	D	321	1/1	0.90	0.10	92,92,92,92	0
2	CD	E	319	1/1	0.91	0.08	50,50,50,50	0
3	NI	H	321	1/1	0.92	0.09	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NI	A	323	1/1	0.92	0.07	81,81,81,81	0
3	NI	H	323	1/1	0.93	0.08	79,79,79,79	0
3	NI	A	322	1/1	0.94	0.08	80,80,80,80	0
2	CD	G	319	1/1	0.95	0.06	40,40,40,40	0
3	NI	B	321	1/1	0.96	0.05	37,37,37,37	0
3	NI	G	321	1/1	0.96	0.05	59,59,59,59	0
3	NI	D	320	1/1	0.97	0.04	53,53,53,53	0
3	NI	E	321	1/1	0.97	0.08	49,49,49,49	0
3	NI	C	321	1/1	0.98	0.04	58,58,58,58	0
2	CD	H	319	1/1	0.98	0.08	50,50,50,50	0
2	CD	F	318	1/1	0.98	0.03	38,38,38,38	0
3	NI	B	320	1/1	0.98	0.04	40,40,40,40	0
2	CD	D	318	1/1	0.99	0.03	39,39,39,39	0
2	CD	D	319	1/1	0.99	0.07	60,60,60,60	0
2	CD	E	318	1/1	0.99	0.03	36,36,36,36	0
2	CD	A	320	1/1	0.99	0.07	50,50,50,50	0
2	CD	E	320	1/1	0.99	0.06	57,57,57,57	0
3	NI	B	322	1/1	0.99	0.04	35,35,35,35	0
2	CD	B	318	1/1	0.99	0.02	33,33,33,33	0
2	CD	F	319	1/1	0.99	0.07	62,62,62,62	0
2	CD	G	318	1/1	0.99	0.03	35,35,35,35	0
2	CD	B	319	1/1	0.99	0.08	53,53,53,53	0
2	CD	G	320	1/1	0.99	0.06	54,54,54,54	0
2	CD	H	318	1/1	0.99	0.03	33,33,33,33	0
2	CD	C	318	1/1	0.99	0.03	41,41,41,41	0
3	NI	H	320	1/1	0.99	0.03	38,38,38,38	0
3	NI	A	321	1/1	0.99	0.03	34,34,34,34	0
2	CD	A	318	1/1	0.99	0.02	32,32,32,32	0
2	CD	C	320	1/1	0.99	0.05	63,63,63,63	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.