



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:12 PM UTC

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

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:

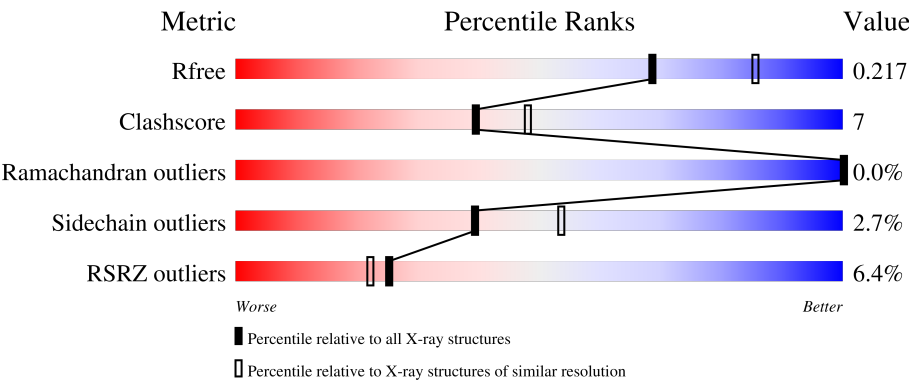
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 $\leq 5\%$. 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	5% 77% 17%
1	B	317	5% 80% 16%
1	C	317	7% 84% 12%
1	D	317	9% 82% 15%
1	E	317	7% 82% 14%

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Mol	Chain	Length	Quality of chain		
1	F	317	4%	83%	13% ..
1	G	317	8%	81%	14% ..
1	H	317	5%	81%	15% ..

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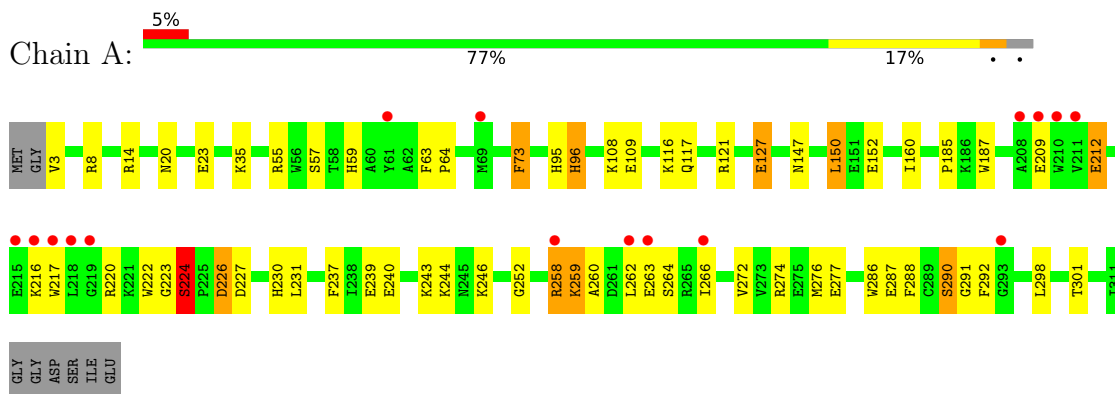
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	159	Total 159	O 159	0	0

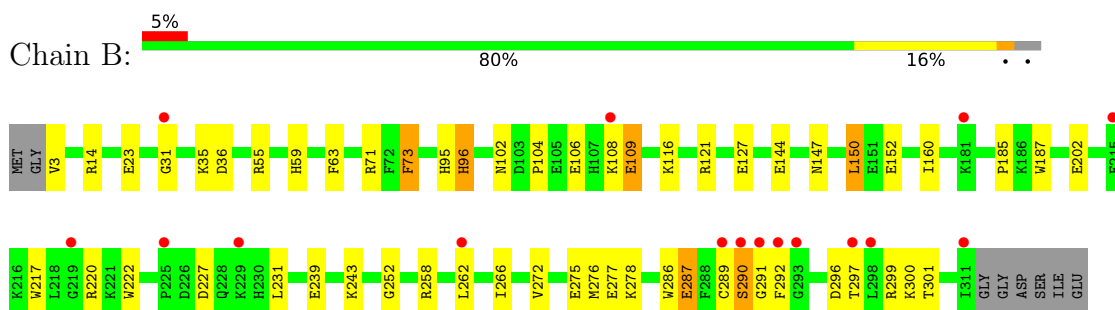
3 Residue-property plots

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.

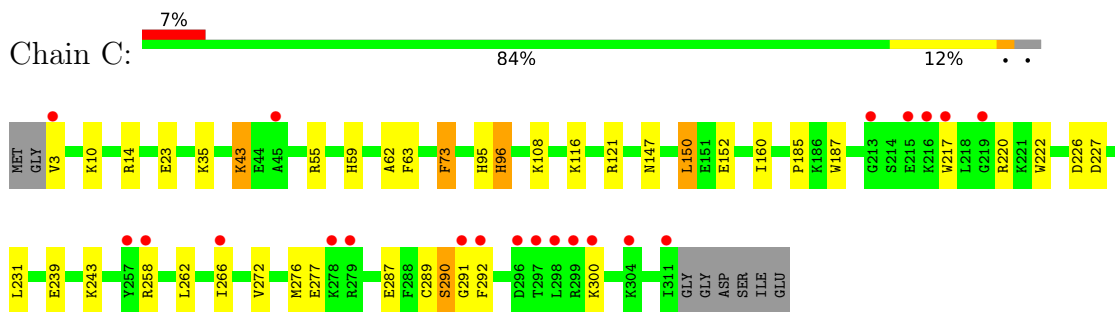
• Molecule 1: Endoglucanase



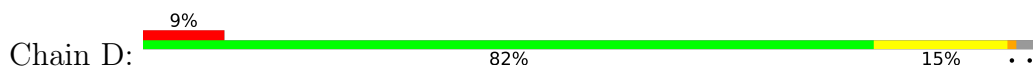
• Molecule 1: Endoglucanase

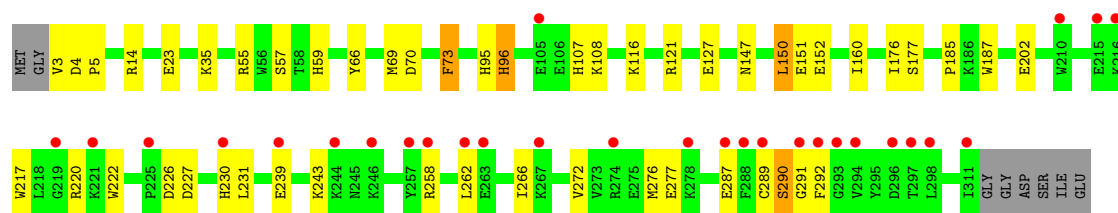


• Molecule 1: Endoglucanase

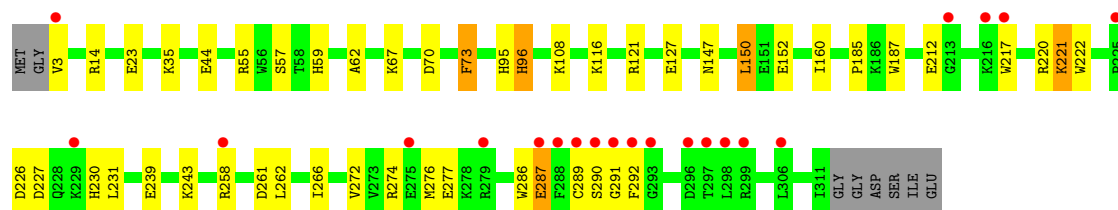
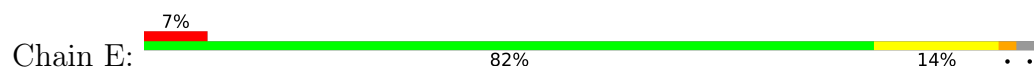


• Molecule 1: Endoglucanase

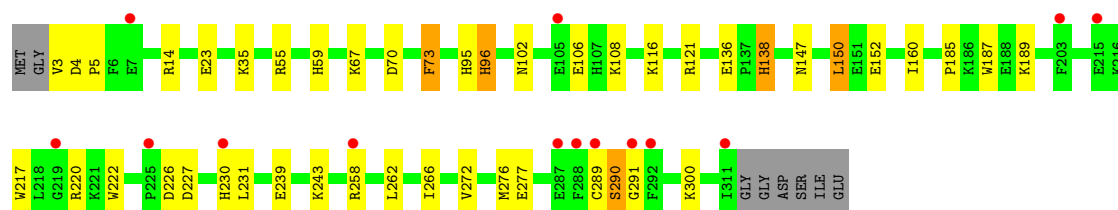
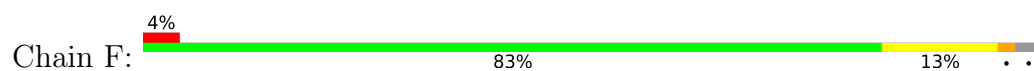




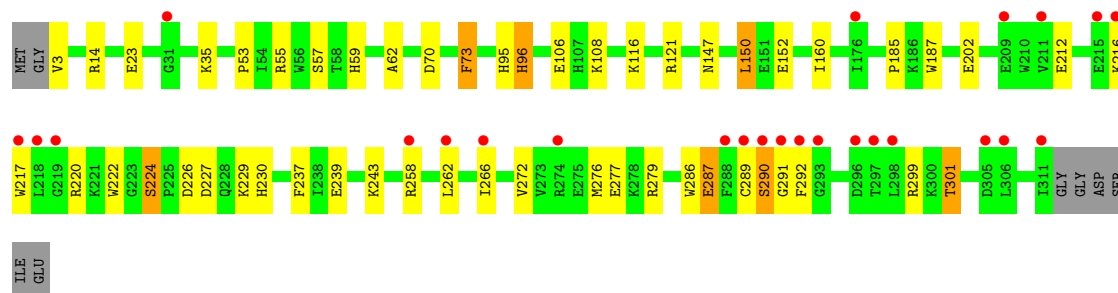
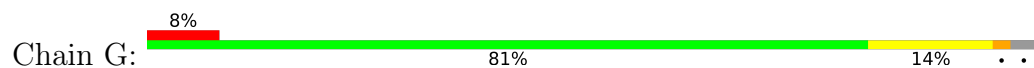
• Molecule 1: Endoglucanase



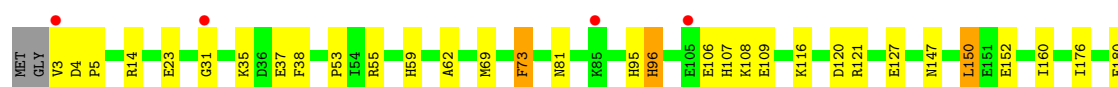
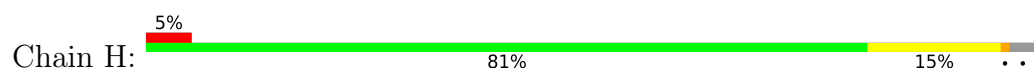
• Molecule 1: Endoglucanase

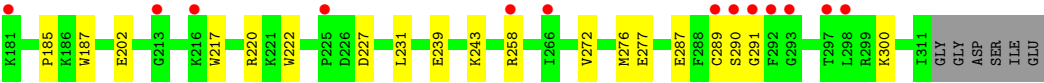


• Molecule 1: Endoglucanase



• Molecule 1: Endoglucanase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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%)	36	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	45
1	B	272/277 (98%)	264 (97%)	8 (3%)	37	51
1	C	272/277 (98%)	265 (97%)	7 (3%)	40	55
1	D	272/277 (98%)	264 (97%)	8 (3%)	37	51
1	E	272/277 (98%)	263 (97%)	9 (3%)	33	45
1	F	272/277 (98%)	267 (98%)	5 (2%)	51	68
1	G	272/277 (98%)	264 (97%)	8 (3%)	37	51
1	H	272/277 (98%)	267 (98%)	5 (2%)	51	68
All	All	2176/2216 (98%)	2117 (97%)	59 (3%)	39	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, 95th 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 ²)	Q<0.9
1	A	309/317 (97%)	0.45	16 (5%)	33	29	21, 38, 66, 121	0
1	B	309/317 (97%)	0.46	16 (5%)	33	29	23, 42, 73, 88	0
1	C	309/317 (97%)	0.66	21 (6%)	23	20	28, 54, 92, 146	0
1	D	309/317 (97%)	0.68	29 (9%)	14	11	22, 49, 99, 131	0
1	E	309/317 (97%)	0.55	21 (6%)	23	20	25, 44, 90, 112	0
1	F	309/317 (97%)	0.63	14 (4%)	38	35	24, 51, 101, 118	0
1	G	309/317 (97%)	0.48	25 (8%)	18	15	23, 41, 77, 114	0
1	H	309/317 (97%)	0.49	17 (5%)	30	27	23, 41, 70, 95	0
All	All	2472/2536 (97%)	0.55	159 (6%)	25	22	21, 44, 87, 146	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	289	CYS	5.7
1	F	289	CYS	5.0
1	G	216	LYS	4.9
1	E	292	PHE	4.9
1	D	219	GLY	4.8
1	E	291	GLY	4.6
1	A	216	LYS	4.6
1	G	289	CYS	4.2
1	C	213	GLY	4.1
1	F	292	PHE	4.1
1	E	288	PHE	4.1
1	D	298	LEU	4.0
1	C	219	GLY	3.9
1	B	289	CYS	3.9
1	C	298	LEU	3.8
1	B	291	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	F	291	GLY	3.8
1	G	291	GLY	3.7
1	G	298	LEU	3.7
1	G	297	THR	3.7
1	A	266	ILE	3.6
1	G	292	PHE	3.5
1	G	290	SER	3.5
1	E	293	GLY	3.4
1	C	311	ILE	3.4
1	H	297	THR	3.3
1	D	297	THR	3.3
1	F	311	ILE	3.3
1	D	257	TYR	3.3
1	A	293	GLY	3.2
1	H	213	GLY	3.2
1	D	262	LEU	3.2
1	G	293	GLY	3.2
1	H	298	LEU	3.2
1	C	299	ARG	3.1
1	B	290	SER	3.1
1	F	288	PHE	3.1
1	H	289	CYS	3.1
1	D	225	PRO	3.1
1	A	215	GLU	3.0
1	A	219	GLY	3.0
1	F	258	ARG	3.0
1	D	311	ILE	3.0
1	F	215	GLU	3.0
1	H	293	GLY	3.0
1	H	105	GLU	3.0
1	D	216	LYS	2.9
1	H	258	ARG	2.9
1	A	258	ARG	2.9
1	C	216	LYS	2.9
1	C	296	ASP	2.9
1	A	218	LEU	2.8
1	D	292	PHE	2.8
1	B	225	PRO	2.8
1	D	215	GLU	2.8
1	B	292	PHE	2.8
1	D	289	CYS	2.8
1	F	225	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	105	GLU	2.7
1	B	108	LYS	2.7
1	G	288	PHE	2.7
1	C	3	VAL	2.7
1	G	296	ASP	2.7
1	D	258	ARG	2.7
1	C	292	PHE	2.6
1	D	288	PHE	2.6
1	C	266	ILE	2.6
1	G	266	ILE	2.6
1	D	274	ARG	2.6
1	G	258	ARG	2.6
1	B	297	THR	2.6
1	E	225	PRO	2.6
1	D	296	ASP	2.5
1	H	181	LYS	2.5
1	D	210	TRP	2.5
1	G	262	LEU	2.5
1	G	219	GLY	2.5
1	D	263	GLU	2.5
1	C	300	LYS	2.5
1	A	208	ALA	2.5
1	D	294	VAL	2.4
1	H	292	PHE	2.4
1	B	181	LYS	2.4
1	H	216	LYS	2.4
1	A	262	LEU	2.4
1	E	299	ARG	2.4
1	E	275	GLU	2.4
1	B	219	GLY	2.4
1	D	278	LYS	2.4
1	B	298	LEU	2.4
1	H	291	GLY	2.4
1	C	297	THR	2.4
1	E	290	SER	2.4
1	B	262	LEU	2.4
1	E	306	LEU	2.4
1	A	217	TRP	2.4
1	C	217	TRP	2.4
1	C	278	LYS	2.3
1	G	274	ARG	2.3
1	G	306	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	210	TRP	2.3
1	C	291	GLY	2.3
1	D	291	GLY	2.3
1	E	213	GLY	2.3
1	H	31	GLY	2.3
1	E	287	GLU	2.3
1	D	239	GLU	2.3
1	B	229	LYS	2.3
1	G	218	LEU	2.3
1	G	31	GLY	2.3
1	E	258	ARG	2.3
1	E	297	THR	2.3
1	F	287	GLU	2.3
1	A	211	VAL	2.3
1	A	61	TYR	2.2
1	F	105	GLU	2.2
1	H	290	SER	2.2
1	C	304	LYS	2.2
1	D	230	HIS	2.2
1	C	257	TYR	2.2
1	E	217	TRP	2.2
1	G	215	GLU	2.2
1	G	211	VAL	2.1
1	G	305	ASP	2.1
1	A	209	GLU	2.1
1	B	215	GLU	2.1
1	E	229	LYS	2.1
1	F	203	PHE	2.1
1	H	85	LYS	2.1
1	H	225	PRO	2.1
1	A	69	MET	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	G	176	ILE	2.1
1	A	263	GLU	2.1
1	G	217	TRP	2.1
1	D	221	LYS	2.1
1	F	7	GLU	2.1
1	F	230	HIS	2.1
1	B	293	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	293	GLY	2.1
1	F	219	GLY	2.1
1	E	298	LEU	2.1
1	B	311	ILE	2.1
1	G	311	ILE	2.1
1	E	3	VAL	2.1
1	B	31	GLY	2.1
1	C	279	ARG	2.1
1	C	215	GLU	2.0
1	G	209	GLU	2.0
1	E	296	ASP	2.0
1	H	266	ILE	2.0
1	C	258	ARG	2.0
1	E	279	ARG	2.0
1	H	3	VAL	2.0
1	D	287	GLU	2.0
1	C	45	ALA	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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 [i](#)

There are no such residues in this entry.