



# Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2026 – 04:28 PM EDT

PDB ID : 9Z0B / pdb\_00009z0b  
Title : Crystal Structure of the Polycaprolactam (Nylon6) and Poly(Hexamethylene Adipamide) (Nylon66) Hydrolase Nyl12 at Cryo Temperature  
Authors : Capra, N.; Meilleur, F.  
Deposited on : 2025-10-31  
Resolution : 1.75 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 Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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

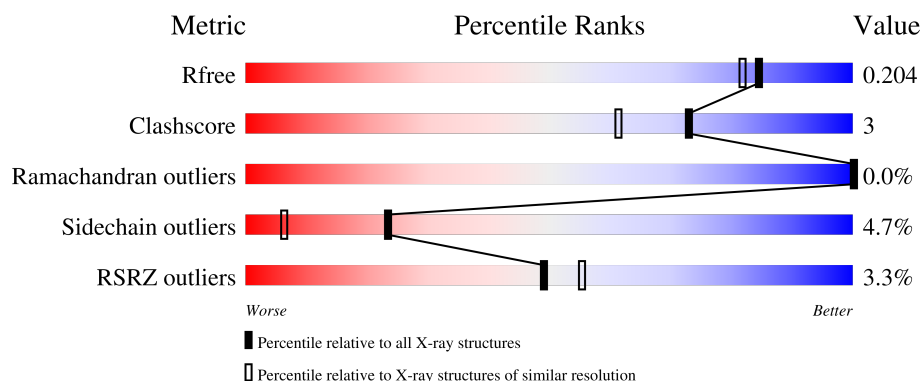
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



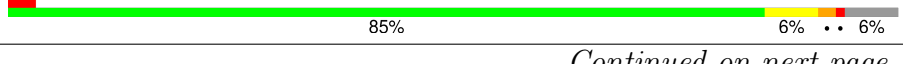
The reported resolution of this entry is 1.75 Å.

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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	328	
1	B	328	
1	C	328	
1	D	328	
1	E	328	

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Mol	Chain	Length	Quality of chain
1	F	328	
1	G	328	
1	H	328	

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
2	CHT	A	401	-	-	X	-
2	CHT	D	401	-	-	X	-
3	ACT	H	401	-	X	X	-
6	EDO	D	402	-	-	X	-
7	PEG	D	403	-	-	X	-

## 2 Entry composition

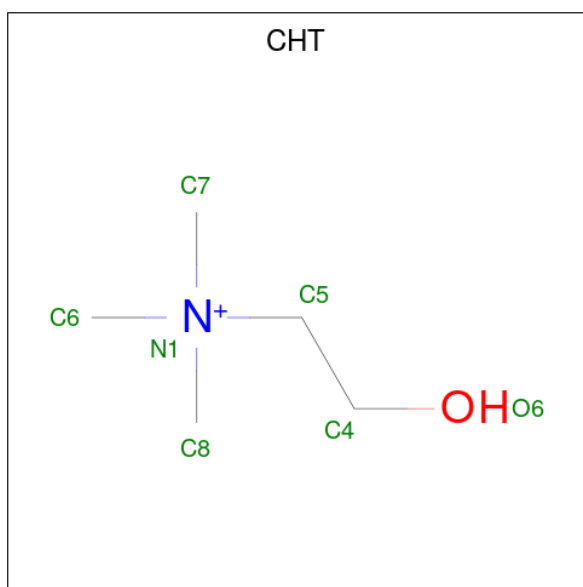
There are 8 unique types of molecules in this entry. The entry contains 19711 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Poly (caprolactam and hexamethylene adipamide) hydrolase Nyl12.

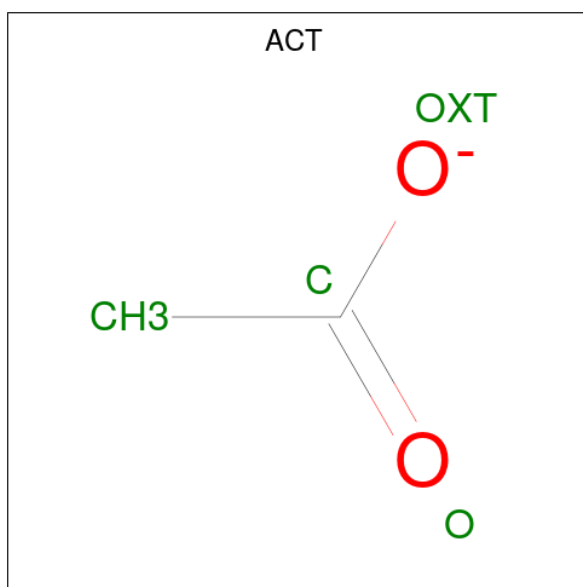
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2367	1521	400	442	4			
1	B	313	Total	C	N	O	S	0	1	0
			2371	1523	401	443	4			
1	C	311	Total	C	N	O	S	0	0	0
			2345	1506	395	440	4			
1	D	304	Total	C	N	O	S	0	0	0
			2282	1466	384	428	4			
1	E	308	Total	C	N	O	S	0	0	0
			2327	1497	393	433	4			
1	F	309	Total	C	N	O	S	0	0	0
			2334	1502	394	434	4			
1	G	312	Total	C	N	O	S	0	0	0
			2353	1510	398	441	4			
1	H	314	Total	C	N	O	S	0	1	0
			2378	1527	402	445	4			

- Molecule 2 is CHOLINE ION (CCD ID: CHT) (formula: C<sub>5</sub>H<sub>14</sub>NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			7	5	1	1		
2	D	1	Total	C	N	O	0	0
			7	5	1	1		
2	G	1	Total	C	N	O	0	0
			7	5	1	1		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula:  $C_2H_3O_2$ ).



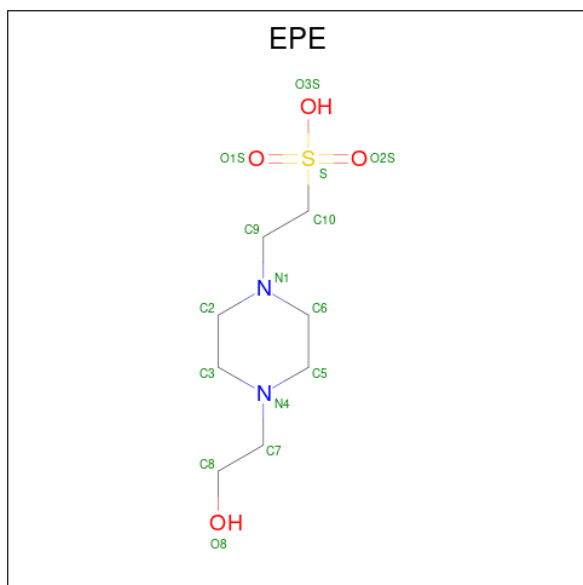
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



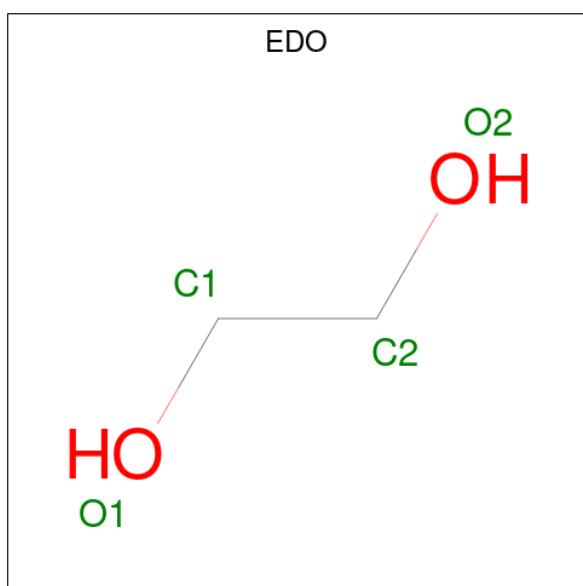
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			7	4	3		
7	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is water.

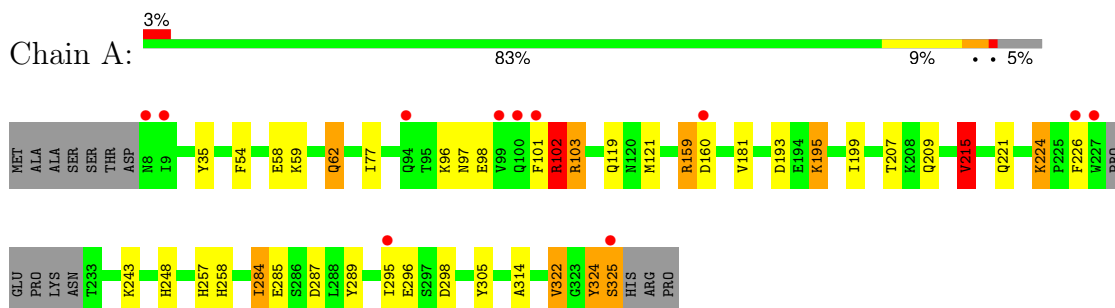
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	116	Total	O	0	2
			118	118		
8	B	101	Total	O	0	0
			101	101		
8	C	110	Total	O	0	0
			110	110		
8	D	81	Total	O	0	0
			81	81		
8	E	108	Total	O	0	1
			109	109		
8	F	111	Total	O	0	1
			112	112		
8	G	88	Total	O	0	0
			88	88		
8	H	116	Total	O	0	0
			116	116		



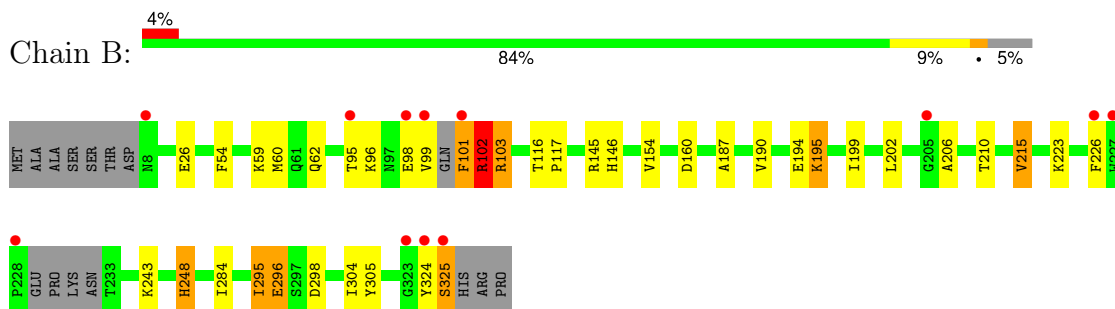
### 3 Residue-property plots [i](#)

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.

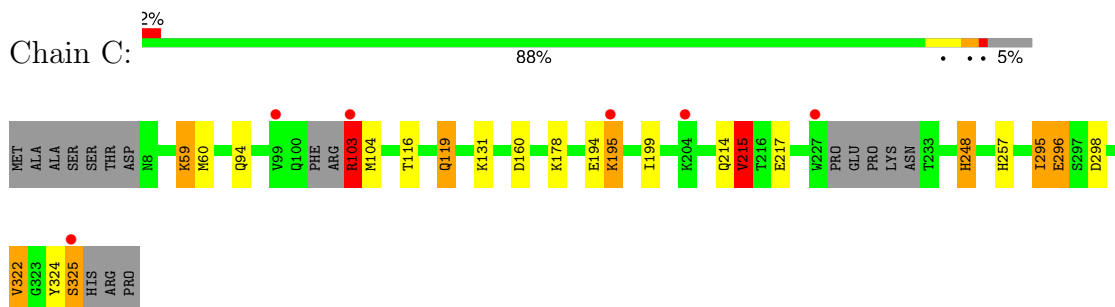
- Molecule 1: Poly (caprolactam and hexamethylene adipamide) hydrolase Nyl12



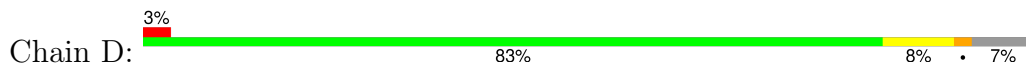
- Molecule 1: Poly (caprolactam and hexamethylene adipamide) hydrolase Nyl12

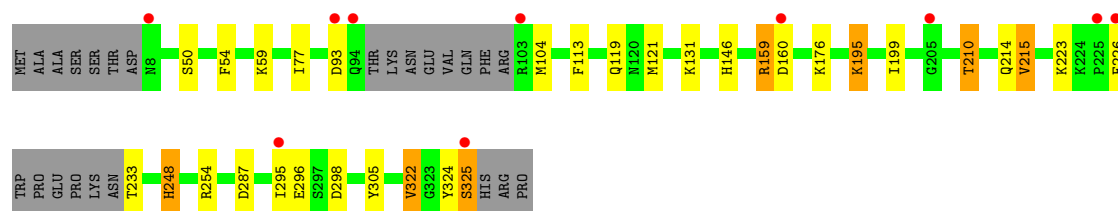


- Molecule 1: Poly (caprolactam and hexamethylene adipamide) hydrolase Nyl12

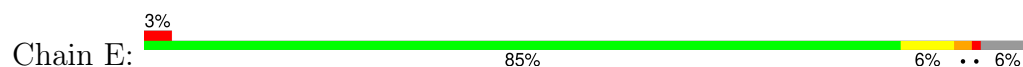


- Molecule 1: Poly (caprolactam and hexamethylene adipamide) hydrolase Nyl12

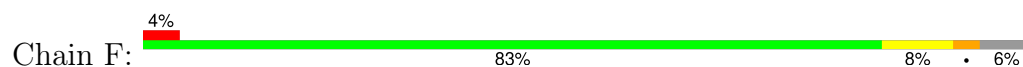




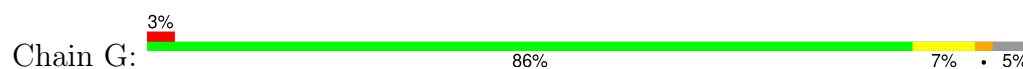
- Molecule 1: Poly (caprolactam and hexamethylene adipamide) hydrolase Nyl12



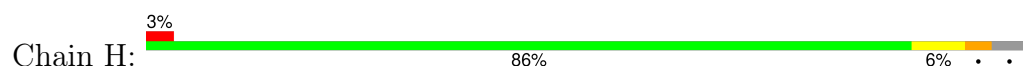
- Molecule 1: Poly (caprolactam and hexamethylene adipamide) hydrolase Nyl12



- Molecule 1: Poly (caprolactam and hexamethylene adipamide) hydrolase Nyl12



- Molecule 1: Poly (caprolactam and hexamethylene adipamide) hydrolase Nyl12



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.62Å 135.41Å 142.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	98.28 – 1.75 98.28 – 1.75	Depositor EDS
% Data completeness (in resolution range)	93.6 (98.28-1.75) 92.5 (98.28-1.75)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, $R_{free}$	0.161 , 0.197 0.171 , 0.204	Depositor DCC
$R_{free}$ test set	10811 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.4	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 34.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	19711	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% 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: EDO, ACT, EPE, GOL, PEG, CHT

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	0.98	1/2415 (0.0%)	1.36	24/3274 (0.7%)
1	B	1.02	2/2418 (0.1%)	1.30	18/3277 (0.5%)
1	C	0.98	1/2391 (0.0%)	1.27	15/3241 (0.5%)
1	D	0.99	0/2326	1.30	19/3152 (0.6%)
1	E	0.99	1/2374 (0.0%)	1.32	19/3217 (0.6%)
1	F	0.99	1/2382 (0.0%)	1.29	21/3229 (0.7%)
1	G	0.98	2/2399 (0.1%)	1.30	20/3251 (0.6%)
1	H	0.97	0/2426	1.28	18/3289 (0.5%)
All	All	0.99	8/19131 (0.0%)	1.30	154/25930 (0.6%)

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	1
1	B	0	3
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	3
1	G	0	1
All	All	0	11

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	295	ILE	CB-CG1	-7.03	1.39	1.53
1	G	248	HIS	CG-CD2	-6.57	1.28	1.35
1	F	295	ILE	CB-CG1	-5.79	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	226	PHE	C-O	5.75	1.35	1.23
1	A	258	HIS	CE1-NE2	5.45	1.38	1.32
1	E	59	LYS	CB-CG	-5.41	1.36	1.52
1	B	248	HIS	ND1-CE1	5.37	1.38	1.32
1	B	284	ILE	CB-CG1	-5.27	1.43	1.53

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	MET	CG-SD-CE	12.75	128.95	100.90
1	H	322	VAL	N-CA-CB	-12.15	96.12	112.28
1	G	322	VAL	N-CA-CB	-11.92	96.43	112.28
1	C	322	VAL	N-CA-CB	-11.86	96.51	112.28
1	F	322	VAL	N-CA-CB	-11.76	96.65	112.28
1	E	322	VAL	N-CA-CB	-11.66	96.77	112.28
1	A	322	VAL	N-CA-CB	-10.89	97.79	112.28
1	D	322	VAL	N-CA-CB	-10.34	98.53	112.28
1	F	121	MET	CG-SD-CE	-9.84	79.26	100.90
1	H	228	PRO	N-CA-CB	9.09	113.00	103.00
1	E	104	MET	CG-SD-CE	-8.94	81.24	100.90
1	E	195	LYS	CG-CD-CE	8.45	130.74	111.30
1	D	210	THR	CA-CB-OG1	-8.17	97.34	109.60
1	G	160	ASP	CB-CA-C	-7.70	96.59	109.99
1	F	217	GLU	CB-CG-CD	7.65	125.60	112.60
1	G	215	VAL	N-CA-CB	-7.65	96.93	110.77
1	G	62	GLN	CG-CD-NE2	-7.60	105.00	116.40
1	F	54	PHE	CA-CB-CG	7.59	121.39	113.80
1	E	54	PHE	CA-CB-CG	7.25	121.05	113.80
1	B	26	GLU	CG-CD-OE2	7.16	134.87	118.40
1	C	215	VAL	N-CA-CB	-7.14	97.84	110.77
1	A	159	ARG	NE-CZ-NH2	7.12	125.61	119.20
1	A	62	GLN	CG-CD-NE2	-7.05	105.83	116.40
1	H	210	THR	CA-CB-OG1	-7.01	99.09	109.60
1	A	287	ASP	CA-CB-CG	6.94	119.54	112.60
1	A	101	PHE	CA-CB-CG	6.88	120.68	113.80
1	A	54	PHE	CA-CB-CG	6.86	120.66	113.80
1	D	160	ASP	CB-CA-C	-6.80	97.96	109.38
1	H	121	MET	CG-SD-CE	6.79	115.84	100.90
1	H	287	ASP	CA-CB-CG	6.75	119.35	112.60
1	B	96	LYS	CA-CB-CG	6.75	127.59	114.10
1	E	215	VAL	CG1-CB-CG2	6.71	125.56	110.80
1	E	160	ASP	CB-CA-C	-6.69	98.13	109.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	18	GLN	OE1-CD-NE2	-6.69	115.91	122.60
1	F	210	THR	CA-CB-OG1	-6.66	99.61	109.60
1	E	215	VAL	N-CA-CB	-6.63	98.77	110.77
1	A	224	LYS	CB-CG-CD	6.58	126.43	111.30
1	G	195	LYS	CG-CD-CE	6.54	126.34	111.30
1	C	195	LYS	CG-CD-CE	6.52	126.30	111.30
1	B	215	VAL	N-CA-CB	-6.47	99.05	110.77
1	G	210	THR	CA-CB-OG1	-6.46	99.91	109.60
1	A	215	VAL	N-CA-CB	-6.44	99.11	110.77
1	H	215	VAL	N-CA-CB	-6.40	99.18	110.77
1	A	159	ARG	CB-CG-CD	-6.39	96.61	111.30
1	D	93	ASP	CA-CB-CG	6.37	118.97	112.60
1	D	121	MET	CG-SD-CE	6.30	114.77	100.90
1	B	54	PHE	CA-CB-CG	6.28	120.08	113.80
1	C	160	ASP	CB-CA-C	-6.28	99.07	109.99
1	D	287	ASP	CA-CB-CG	6.24	118.84	112.60
1	E	64	GLU	CB-CG-CD	-6.24	102.00	112.60
1	B	243	LYS	CB-CG-CD	6.23	125.64	111.30
1	B	62	GLN	CG-CD-NE2	-6.22	107.06	116.40
1	A	215	VAL	CG1-CB-CG2	6.17	124.38	110.80
1	F	287	ASP	CA-CB-CG	6.10	118.70	112.60
1	D	215	VAL	N-CA-CB	-6.10	99.74	110.77
1	E	296	GLU	N-CA-CB	6.08	119.59	110.22
1	H	160	ASP	CB-CA-C	-6.06	99.20	109.38
1	A	160	ASP	CB-CA-C	-6.05	99.22	109.38
1	G	59	LYS	N-CA-CB	-6.04	101.24	110.12
1	E	210	THR	CA-CB-OG1	-6.02	100.57	109.60
1	B	210	THR	CA-CB-OG1	-6.01	100.58	109.60
1	A	322	VAL	CA-CB-CG1	5.99	120.58	110.40
1	B	59	LYS	N-CA-CB	-5.99	101.00	110.22
1	G	194	GLU	CB-CG-CD	5.97	122.75	112.60
1	A	103	ARG	CD-NE-CZ	5.95	132.73	124.40
1	F	224	LYS	CG-CD-CE	-5.92	97.69	111.30
1	B	215	VAL	CA-CB-CG1	5.90	120.42	110.40
1	G	72	PHE	CA-CB-CG	5.87	119.67	113.80
1	B	194	GLU	CB-CG-CD	5.84	122.53	112.60
1	D	121	MET	CA-CB-CG	-5.83	102.43	114.10
1	D	146	HIS	CB-CG-CD2	-5.83	123.63	131.20
1	C	215	VAL	CG1-CB-CG2	5.82	123.59	110.80
1	B	146	HIS	CA-CB-CG	-5.80	108.00	113.80
1	A	102	ARG	NE-CZ-NH2	5.80	124.42	119.20
1	F	322	VAL	CA-CB-CG1	5.78	120.23	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	214	GLN	N-CA-CB	5.77	118.38	110.01
1	G	103	ARG	CG-CD-NE	-5.75	99.36	112.00
1	D	215	VAL	CG1-CB-CG2	5.74	123.43	110.80
1	E	160	ASP	N-CA-CB	-5.74	102.96	110.88
1	C	248	HIS	CB-CG-CD2	-5.72	123.77	131.20
1	D	159	ARG	CB-CG-CD	-5.71	98.16	111.30
1	F	195	LYS	CG-CD-CE	5.69	124.40	111.30
1	F	194	GLU	CB-CG-CD	5.69	122.28	112.60
1	C	194	GLU	CB-CG-CD	5.67	122.25	112.60
1	H	322	VAL	CA-CB-CG1	5.66	120.02	110.40
1	D	160	ASP	N-CA-CB	-5.66	103.08	110.88
1	F	146	HIS	CB-CG-CD2	-5.65	123.85	131.20
1	B	62	GLN	OE1-CD-NE2	5.64	128.24	122.60
1	H	195	LYS	CG-CD-CE	5.63	124.25	111.30
1	H	102	ARG	NE-CZ-NH2	5.62	124.26	119.20
1	E	194	GLU	CB-CG-CD	5.61	122.14	112.60
1	F	214	GLN	N-CA-CB	5.61	118.14	110.01
1	E	160	ASP	CA-CB-CG	5.60	118.20	112.60
1	B	215	VAL	CG1-CB-CG2	5.56	123.03	110.80
1	D	322	VAL	CA-CB-CG1	5.55	119.84	110.40
1	C	217	GLU	CG-CD-OE1	5.53	131.11	118.40
1	G	226	PHE	CA-C-O	-5.53	111.41	120.80
1	G	215	VAL	CG1-CB-CG2	5.52	122.94	110.80
1	B	101	PHE	CB-CA-C	5.50	120.54	110.10
1	H	93	ASP	CA-CB-CG	5.50	118.09	112.60
1	G	116	THR	CA-CB-OG1	-5.49	101.36	109.60
1	H	160	ASP	N-CA-CB	-5.49	103.30	110.88
1	F	101	PHE	CA-CB-CG	5.48	119.28	113.80
1	A	224	LYS	CA-CB-CG	5.47	125.05	114.10
1	F	160	ASP	CB-CA-C	-5.47	100.47	109.99
1	B	296	GLU	N-CA-CB	5.44	118.60	110.22
1	A	193	ASP	CA-CB-CG	5.43	118.03	112.60
1	G	322	VAL	CG1-CB-CG2	5.43	122.74	110.80
1	E	59	LYS	N-CA-CB	-5.41	101.89	110.22
1	A	215	VAL	CA-CB-CG1	5.40	119.58	110.40
1	H	215	VAL	CA-CB-CG1	5.40	119.58	110.40
1	A	98	GLU	CG-CD-OE2	-5.38	106.03	118.40
1	H	59	LYS	CA-CB-CG	5.35	124.80	114.10
1	D	248	HIS	CB-CG-CD2	-5.35	124.25	131.20
1	E	54	PHE	N-CA-CB	-5.32	101.74	110.68
1	B	96	LYS	CB-CA-C	-5.32	101.96	110.79
1	E	322	VAL	CA-CB-CG1	5.32	119.44	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	104	MET	CG-SD-CE	-5.30	89.23	100.90
1	G	160	ASP	N-CA-CB	-5.30	102.90	110.80
1	H	296	GLU	N-CA-CB	5.30	118.38	110.22
1	A	160	ASP	N-CA-CB	-5.30	103.57	110.88
1	A	101	PHE	N-CA-CB	-5.29	101.04	109.19
1	H	214	GLN	N-CA-CB	5.25	117.63	110.01
1	A	324	TYR	CA-C-N	5.25	131.15	121.70
1	A	324	TYR	C-N-CA	5.25	131.15	121.70
1	F	224	LYS	CB-CG-CD	5.24	123.36	111.30
1	E	224	LYS	CA-CB-CG	5.24	124.58	114.10
1	E	116	THR	CA-CB-OG1	-5.24	101.75	109.60
1	H	160	ASP	CA-CB-CG	5.23	117.83	112.60
1	B	103	ARG	CD-NE-CZ	5.23	131.72	124.40
1	D	54	PHE	CA-CB-CG	5.22	119.02	113.80
1	C	116	THR	CA-CB-OG1	-5.21	101.79	109.60
1	H	54	PHE	N-CA-CB	-5.21	102.60	110.77
1	G	93	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	59	LYS	N-CA-CB	-5.17	102.26	110.22
1	C	214	GLN	N-CA-CB	5.16	117.49	110.01
1	C	322	VAL	CA-CB-CG1	5.16	119.17	110.40
1	C	296	GLU	N-CA-CB	5.15	118.14	110.22
1	F	94	GLN	CB-CA-C	-5.13	100.34	110.10
1	D	59	LYS	N-CA-CB	-5.12	102.33	110.22
1	F	296	GLU	N-CA-CB	5.11	118.09	110.22
1	G	215	VAL	CA-CB-CG1	5.10	119.08	110.40
1	F	59	LYS	N-CA-CB	-5.10	102.36	110.22
1	C	217	GLU	CG-CD-OE2	-5.09	106.70	118.40
1	C	119	GLN	CB-CG-CD	5.08	121.24	112.60
1	G	322	VAL	CB-CA-C	5.08	118.30	111.85
1	F	59	LYS	CA-CB-CG	5.08	124.26	114.10
1	C	59	LYS	CA-CB-CG	5.07	124.24	114.10
1	G	100	GLN	N-CA-CB	5.06	118.88	110.63
1	F	102	ARG	NE-CZ-NH1	-5.04	116.46	121.50
1	B	160	ASP	CA-CB-CG	5.02	117.62	112.60
1	D	214	GLN	CB-CA-C	-5.01	103.02	110.88
1	D	195	LYS	CG-CD-CE	5.00	122.81	111.30
1	G	62	GLN	OE1-CD-NE2	5.00	127.60	122.60

There are no chirality outliers.

All (11) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	102	ARG	Sidechain
1	B	102	ARG	Sidechain
1	B	103	ARG	Sidechain
1	B	145	ARG	Sidechain
1	C	103	ARG	Sidechain
1	D	254	ARG	Sidechain
1	E	103	ARG	Sidechain
1	F	102	ARG	Sidechain
1	F	103	ARG	Sidechain
1	F	118	ARG	Sidechain
1	G	103	ARG	Sidechain

## 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	2367	0	2379	24	0
1	B	2371	0	2376	16	0
1	C	2345	0	2356	8	0
1	D	2282	0	2297	14	0
1	E	2327	0	2337	12	0
1	F	2334	0	2344	10	0
1	G	2353	0	2369	12	0
1	H	2378	0	2384	18	0
2	A	7	0	14	6	0
2	D	7	0	14	6	0
2	G	7	0	14	1	0
3	A	4	0	3	0	0
3	H	4	0	3	4	0
4	C	15	0	18	0	0
4	E	15	0	18	1	0
4	F	30	0	36	1	0
5	C	6	0	8	1	0
5	D	6	0	8	1	0
6	D	4	0	6	4	0
7	D	14	0	20	8	0
8	A	118	0	0	10	0
8	B	101	0	0	2	0
8	C	110	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	81	0	0	4	0
8	E	109	0	0	2	0
8	F	112	0	0	4	0
8	G	88	0	0	2	0
8	H	116	0	0	3	0
All	All	19711	0	19004	122	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (122) 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:B:195:LYS:O	1:E:195:LYS:HE3	1.59	1.02
2:D:401:CHT:H63	7:D:403:PEG:H42	1.02	1.01
2:D:401:CHT:C6	7:D:403:PEG:H42	1.95	0.97
1:G:104:MET:HE3	1:G:105:PRO:HD2	1.47	0.96
2:D:401:CHT:H63	7:D:403:PEG:C4	1.96	0.95
7:D:403:PEG:H12	8:D:538:HOH:O	1.67	0.94
1:H:95:THR:HG22	1:H:102:ARG:HH11	1.45	0.81
1:D:113:PHE:HB3	7:D:403:PEG:H11	1.67	0.77
1:A:221:GLN:HG2	8:A:587:HOH:O	1.84	0.77
1:A:103:ARG:CZ	8:A:502:HOH:O	2.34	0.76
1:A:195:LYS:HE2	8:H:606:HOH:O	1.87	0.75
1:F:220:GLN:HG2	8:F:502:HOH:O	1.89	0.73
1:H:100:GLN:CD	1:H:100:GLN:H	1.95	0.72
5:D:405:GOL:H2	8:D:519:HOH:O	1.90	0.71
1:H:156:LYS:NZ	3:H:401:ACT:H3	2.05	0.71
1:G:101:PHE:CZ	1:G:104:MET:HG2	2.27	0.69
1:A:35:TYR:OH	1:A:96:LYS:HE2	1.94	0.67
1:G:101:PHE:HZ	1:G:104:MET:HG2	1.59	0.67
1:B:95:THR:HG22	1:B:102:ARG:HD2	1.77	0.65
1:B:295:ILE:HD13	4:E:401:EPE:H71	1.79	0.65
1:G:104:MET:CE	1:G:105:PRO:HD2	2.25	0.64
1:H:95:THR:CG2	1:H:102:ARG:HH11	2.09	0.64
1:H:156:LYS:HZ3	3:H:401:ACT:H3	1.64	0.63
1:C:248:HIS:HD2	8:C:525:HOH:O	1.82	0.62
1:A:77:ILE:HG22	2:A:401:CHT:O6	2.00	0.62
1:A:97:ASN:ND2	1:A:102:ARG:HD3	2.16	0.60
1:G:104:MET:HE3	1:G:105:PRO:CD	2.29	0.59
1:F:104:MET:HA	1:F:104:MET:HE2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:248:HIS:HD2	8:G:528:HOH:O	1.85	0.58
1:H:95:THR:HG21	8:H:609:HOH:O	2.04	0.58
1:D:248:HIS:HD2	8:D:525:HOH:O	1.87	0.57
1:B:248:HIS:HE1	1:B:298:ASP:OD1	1.87	0.57
1:H:227:TRP:O	1:H:228:PRO:CB	2.53	0.56
1:A:305:TYR:CD1	1:H:215:VAL:HG22	2.40	0.56
2:A:401:CHT:C4	8:A:593:HOH:O	2.52	0.56
1:C:178:LYS:HE3	8:C:534:HOH:O	2.05	0.56
1:A:248:HIS:HD2	8:A:517:HOH:O	1.89	0.55
1:F:220:GLN:NE2	8:F:502:HOH:O	2.33	0.55
1:G:101:PHE:HZ	1:G:104:MET:CG	2.20	0.55
1:B:248:HIS:HD2	8:B:433:HOH:O	1.90	0.55
5:C:402:GOL:H2	8:C:502:HOH:O	2.07	0.54
1:E:248:HIS:HD2	8:E:510:HOH:O	1.89	0.54
1:H:101:PHE:O	1:H:103:ARG:NE	2.35	0.54
1:D:159:ARG:HD3	1:D:226:PHE:O	2.08	0.53
1:E:104:MET:HE2	1:E:104:MET:HA	1.89	0.53
1:A:103:ARG:NH2	8:A:502:HOH:O	2.40	0.53
1:A:77:ILE:N	2:A:401:CHT:O6	2.30	0.53
1:H:248:HIS:HE1	1:H:298:ASP:OD1	1.92	0.53
1:H:156:LYS:HD2	3:H:401:ACT:C	2.39	0.52
2:D:401:CHT:H62	8:D:577:HOH:O	2.09	0.52
1:B:223:LYS:HE3	1:B:226:PHE:CE1	2.44	0.52
1:C:248:HIS:HE1	1:C:298:ASP:OD1	1.93	0.52
1:A:248:HIS:HE1	1:A:298:ASP:OD1	1.93	0.52
1:C:104:MET:HA	1:C:104:MET:HE2	1.90	0.52
1:A:215:VAL:HG22	1:H:305:TYR:CD1	2.44	0.52
1:A:243:LYS:HE2	1:A:289:TYR:CE2	2.45	0.52
1:F:248:HIS:HD2	8:F:525:HOH:O	1.92	0.52
1:G:248:HIS:HE1	1:G:298:ASP:OD1	1.93	0.52
1:D:104:MET:HA	1:D:104:MET:HE2	1.93	0.51
1:A:77:ILE:H	2:A:401:CHT:C4	2.23	0.51
1:E:146:HIS:HE1	8:E:602:HOH:O	1.93	0.51
1:C:215:VAL:HG22	1:D:305:TYR:CD1	2.46	0.51
1:H:116:THR:OG1	3:H:401:ACT:H1	2.10	0.51
1:A:159:ARG:HD3	1:A:226:PHE:O	2.11	0.51
1:B:305:TYR:CD1	1:E:215:VAL:HG22	2.46	0.51
1:D:50:SER:O	7:D:403:PEG:H31	2.11	0.50
1:C:103:ARG:HD2	1:C:103:ARG:N	2.26	0.50
1:F:248:HIS:HE1	1:F:298:ASP:OD1	1.94	0.50
1:G:176:LYS:NZ	8:G:502:HOH:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:324:TYR:O	1:G:325:SER:HB2	2.10	0.50
1:D:248:HIS:HE1	1:D:298:ASP:OD1	1.95	0.50
1:A:221:GLN:CG	8:A:587:HOH:O	2.52	0.50
1:B:190:VAL:HG11	1:B:202:LEU:HG	1.94	0.50
1:H:248:HIS:HD2	8:H:513:HOH:O	1.94	0.50
1:D:176:LYS:NZ	6:D:402:EDO:H21	2.27	0.50
1:D:324:TYR:O	1:D:325:SER:HB2	2.12	0.50
1:E:248:HIS:HE1	1:E:298:ASP:OD1	1.95	0.49
2:A:401:CHT:H63	8:A:593:HOH:O	2.12	0.49
4:F:402:EPE:H81	8:F:555:HOH:O	2.13	0.49
1:E:324:TYR:O	1:E:325:SER:HB2	2.13	0.48
1:A:97:ASN:CG	1:A:102:ARG:HD3	2.39	0.48
1:A:103:ARG:NE	8:A:502:HOH:O	2.46	0.48
1:H:324:TYR:O	1:H:325:SER:HB2	2.13	0.48
1:F:209:GLN:HE21	1:F:213:GLN:NE2	2.12	0.48
1:B:116:THR:HB	1:B:117:PRO:HD3	1.97	0.47
1:D:176:LYS:NZ	6:D:402:EDO:C2	2.78	0.47
1:A:324:TYR:O	1:A:325:SER:HB2	2.14	0.47
2:D:401:CHT:H83	2:D:401:CHT:HC42	1.73	0.47
1:B:324:TYR:O	1:B:325:SER:HB2	2.13	0.46
1:B:202:LEU:HD13	1:B:206:ALA:HB3	1.98	0.46
1:F:324:TYR:O	1:F:325:SER:HB2	2.15	0.46
1:A:207:THR:OG1	1:A:209:GLN:HG2	2.16	0.45
1:A:284:ILE:HG13	1:A:285:GLU:N	2.32	0.45
1:C:324:TYR:O	1:C:325:SER:HB2	2.15	0.45
1:D:77:ILE:HB	2:D:401:CHT:HC42	1.99	0.44
2:A:401:CHT:HC42	8:A:593:HOH:O	2.17	0.44
1:B:304:ILE:HD11	1:E:271:LEU:HD12	1.99	0.44
2:G:401:CHT:O6	2:G:401:CHT:H73	2.17	0.44
1:D:176:LYS:HZ1	6:D:402:EDO:H21	1.82	0.44
1:A:221:GLN:CD	8:A:587:HOH:O	2.61	0.43
1:B:102:ARG:HD2	1:B:102:ARG:HH21	1.70	0.43
1:D:233:THR:OG1	7:D:403:PEG:C2	2.66	0.43
1:H:104:MET:HA	1:H:104:MET:HE2	2.01	0.43
1:C:60:MET:HE3	8:C:575:HOH:O	2.18	0.43
1:E:157:LEU:H	1:E:157:LEU:HD23	1.85	0.42
1:F:221:GLN:OE1	1:F:224:LYS:NZ	2.51	0.42
1:A:58:GLU:O	1:A:62:GLN:HG3	2.19	0.42
1:B:60:MET:HE3	8:B:478:HOH:O	2.19	0.42
1:D:176:LYS:HZ1	6:D:402:EDO:C2	2.33	0.42
1:E:121:MET:H	1:E:121:MET:HE2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:101:PHE:CZ	1:G:104:MET:SD	3.13	0.42
1:G:104:MET:HE3	1:G:104:MET:HA	2.03	0.41
7:D:403:PEG:H41	7:D:403:PEG:H21	1.52	0.41
1:B:98:GLU:HB3	1:B:101:PHE:CD1	2.56	0.41
1:F:225:PRO:HB2	1:F:228:PRO:HB3	2.03	0.41
1:E:217:GLU:HG3	1:E:221:GLN:NE2	2.36	0.41
1:F:174:ILE:HD12	1:F:174:ILE:N	2.36	0.41
1:A:181:VAL:HG11	1:A:314:ALA:HA	2.03	0.40
1:H:157:LEU:HD23	1:H:157:LEU:H	1.86	0.40
1:H:223:LYS:HB3	1:H:223:LYS:HE3	1.88	0.40
1:B:154:VAL:HA	1:B:187:ALA:O	2.22	0.40
1:E:154:VAL:HA	1:E:187:ALA:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	309/328 (94%)	303 (98%)	6 (2%)	0	100	100
1	B	308/328 (94%)	300 (97%)	7 (2%)	1 (0%)	36	21
1	C	305/328 (93%)	298 (98%)	7 (2%)	0	100	100
1	D	298/328 (91%)	293 (98%)	5 (2%)	0	100	100
1	E	302/328 (92%)	295 (98%)	7 (2%)	0	100	100
1	F	303/328 (92%)	297 (98%)	6 (2%)	0	100	100
1	G	308/328 (94%)	301 (98%)	7 (2%)	0	100	100
1	H	311/328 (95%)	304 (98%)	7 (2%)	0	100	100
All	All	2444/2624 (93%)	2391 (98%)	52 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	102	ARG

### 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	245/258 (95%)	234 (96%)	11 (4%)	24	7
1	B	245/258 (95%)	238 (97%)	7 (3%)	37	17
1	C	243/258 (94%)	230 (95%)	13 (5%)	20	5
1	D	236/258 (92%)	225 (95%)	11 (5%)	23	6
1	E	240/258 (93%)	231 (96%)	9 (4%)	29	10
1	F	241/258 (93%)	229 (95%)	12 (5%)	22	5
1	G	244/258 (95%)	230 (94%)	14 (6%)	18	4
1	H	246/258 (95%)	232 (94%)	14 (6%)	18	4
All	All	1940/2064 (94%)	1849 (95%)	91 (5%)	23	6

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	A	195	LYS
1	A	199	ILE
1	A	215	VAL
1	A	224	LYS
1	A	257	HIS
1	A	284	ILE
1	A	295	ILE
1	A	296	GLU
1	A	322	VAL
1	A	325	SER
1	B	99	VAL
1	B	195	LYS
1	B	199	ILE
1	B	215	VAL

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Mol	Chain	Res	Type
1	B	295	ILE
1	B	296	GLU
1	B	325	SER
1	C	59	LYS
1	C	94	GLN
1	C	103	ARG
1	C	119	GLN
1	C	131	LYS
1	C	195	LYS
1	C	199	ILE
1	C	215	VAL
1	C	257	HIS
1	C	295	ILE
1	C	296	GLU
1	C	322	VAL
1	C	325	SER
1	D	119	GLN
1	D	131	LYS
1	D	195	LYS
1	D	199	ILE
1	D	210	THR
1	D	215	VAL
1	D	223	LYS
1	D	295	ILE
1	D	296	GLU
1	D	322	VAL
1	D	325	SER
1	E	121	MET
1	E	195	LYS
1	E	199	ILE
1	E	215	VAL
1	E	224	LYS
1	E	295	ILE
1	E	296	GLU
1	E	322	VAL
1	E	325	SER
1	F	102	ARG
1	F	103	ARG
1	F	121	MET
1	F	131	LYS
1	F	195	LYS
1	F	199	ILE

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Mol	Chain	Res	Type
1	F	223	LYS
1	F	257	HIS
1	F	295	ILE
1	F	296	GLU
1	F	322	VAL
1	F	325	SER
1	G	102	ARG
1	G	104	MET
1	G	119	GLN
1	G	131	LYS
1	G	195	LYS
1	G	199	ILE
1	G	204	LYS
1	G	210	THR
1	G	215	VAL
1	G	223	LYS
1	G	295	ILE
1	G	296	GLU
1	G	322	VAL
1	G	325	SER
1	H	59	LYS
1	H	95	THR
1	H	100	GLN
1	H	103	ARG
1	H	119	GLN
1	H	131	LYS
1	H	195	LYS
1	H	199	ILE
1	H	215	VAL
1	H	223	LYS
1	H	224	LYS
1	H	296	GLU
1	H	322	VAL
1	H	325	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	18	GLN
1	A	41	GLN
1	A	248	HIS

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Mol	Chain	Res	Type
1	A	251	GLN
1	A	265	HIS
1	B	18	GLN
1	B	41	GLN
1	B	94	GLN
1	B	248	HIS
1	B	265	HIS
1	C	11	HIS
1	C	41	GLN
1	C	94	GLN
1	C	214	GLN
1	C	248	HIS
1	D	11	HIS
1	D	41	GLN
1	D	47	GLN
1	D	130	GLN
1	D	213	GLN
1	D	221	GLN
1	D	248	HIS
1	E	8	ASN
1	E	11	HIS
1	E	18	GLN
1	E	41	GLN
1	E	119	GLN
1	E	146	HIS
1	E	248	HIS
1	F	8	ASN
1	F	11	HIS
1	F	41	GLN
1	F	62	GLN
1	F	100	GLN
1	F	209	GLN
1	F	213	GLN
1	F	214	GLN
1	F	248	HIS
1	G	8	ASN
1	G	11	HIS
1	G	41	GLN
1	G	214	GLN
1	G	248	HIS
1	H	8	ASN
1	H	11	HIS

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Mol	Chain	Res	Type
1	H	41	GLN
1	H	100	GLN
1	H	248	HIS

### 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](#)

14 ligands 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$
7	PEG	D	404	-	6,6,6	0.51	0	5,5,5	0.38	0
2	CHT	G	401	-	6,6,6	1.57	2 (33%)	8,8,8	1.44	2 (25%)
4	EPE	E	401	-	15,15,15	0.76	0	19,20,20	1.05	3 (15%)
4	EPE	F	402	-	15,15,15	0.90	1 (6%)	19,20,20	1.41	3 (15%)
3	ACT	H	401	-	3,3,3	2.34	1 (33%)	3,3,3	2.34	2 (66%)
3	ACT	A	402	-	3,3,3	1.43	0	3,3,3	0.53	0
4	EPE	F	401	-	15,15,15	1.00	1 (6%)	19,20,20	1.69	3 (15%)
5	GOL	D	405	-	5,5,5	0.26	0	5,5,5	0.66	0
6	EDO	D	402	-	3,3,3	0.42	0	2,2,2	0.59	0
5	GOL	C	402	-	5,5,5	0.43	0	5,5,5	1.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	CHT	D	401	-	6,6,6	1.68	2 (33%)	8,8,8	1.80	2 (25%)
2	CHT	A	401	-	6,6,6	0.85	0	8,8,8	1.31	2 (25%)
7	PEG	D	403	-	6,6,6	0.24	0	5,5,5	0.45	0
4	EPE	C	401	-	15,15,15	0.67	0	19,20,20	1.36	3 (15%)

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
7	PEG	D	404	-	-	2/4/4/4	-
4	EPE	E	401	-	-	1/9/19/19	0/1/1/1
2	CHT	G	401	-	-	1/4/4/4	-
4	EPE	F	402	-	-	0/9/19/19	0/1/1/1
4	EPE	F	401	-	-	2/9/19/19	0/1/1/1
5	GOL	D	405	-	-	3/4/4/4	-
6	EDO	D	402	-	-	1/1/1/1	-
5	GOL	C	402	-	-	2/4/4/4	-
2	CHT	D	401	-	-	3/4/4/4	-
2	CHT	A	401	-	-	4/4/4/4	-
7	PEG	D	403	-	-	4/4/4/4	-
4	EPE	C	401	-	-	1/9/19/19	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	401	ACT	CH3-C	3.56	1.63	1.49
2	G	401	CHT	C7-N1	3.10	1.59	1.50
4	F	402	EPE	O3S-S	3.08	1.58	1.47
4	F	401	EPE	O3S-S	3.06	1.58	1.47
2	D	401	CHT	C8-N1	2.72	1.57	1.50
2	D	401	CHT	C6-N1	2.64	1.57	1.50
2	G	401	CHT	O6-C4	2.00	1.52	1.42

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	401	EPE	O3S-S-C10	-4.00	98.17	106.00
2	D	401	CHT	C7-N1-C5	-3.58	95.67	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	401	EPE	O3S-S-O2S	3.37	119.84	111.40
4	F	401	EPE	O2S-S-C10	-3.31	101.73	106.73
4	F	401	EPE	O3S-S-C10	-3.27	99.61	106.00
3	H	401	ACT	O-C-CH3	-3.03	110.11	122.53
2	D	401	CHT	C8-N1-C6	2.74	116.16	108.98
3	H	401	ACT	OXT-C-CH3	2.67	126.25	115.05
2	A	401	CHT	C6-N1-C5	2.59	120.22	109.91
4	C	401	EPE	O3S-S-O1S	2.43	117.48	111.40
4	F	402	EPE	O3S-S-C10	2.39	110.68	106.00
2	G	401	CHT	C6-N1-C5	-2.37	100.48	109.91
4	F	402	EPE	O1S-S-C10	-2.36	103.16	106.73
4	E	401	EPE	O3S-S-O2S	2.31	117.19	111.40
4	E	401	EPE	O3S-S-O1S	-2.24	105.79	111.40
2	G	401	CHT	C7-N1-C5	2.18	118.59	109.91
4	F	402	EPE	C2-C3-N4	-2.14	106.33	110.65
4	C	401	EPE	C8-C7-N4	2.09	120.79	113.44
4	E	401	EPE	O3S-S-C10	-2.08	101.93	106.00
2	A	401	CHT	C7-N1-C6	-2.08	103.51	108.98

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	CHT	O6-C4-C5-N1
4	C	401	EPE	C8-C7-N4-C3
4	F	401	EPE	C10-C9-N1-C6
5	C	402	GOL	O1-C1-C2-C3
5	D	405	GOL	O1-C1-C2-C3
7	D	404	PEG	O2-C3-C4-O4
7	D	403	PEG	C4-C3-O2-C2
7	D	403	PEG	O2-C3-C4-O4
7	D	404	PEG	O1-C1-C2-O2
5	C	402	GOL	O1-C1-C2-O2
5	D	405	GOL	O1-C1-C2-O2
2	D	401	CHT	C4-C5-N1-C8
4	E	401	EPE	N4-C7-C8-O8
5	D	405	GOL	O2-C2-C3-O3
7	D	403	PEG	O1-C1-C2-O2
4	F	401	EPE	S-C10-C9-N1
2	A	401	CHT	C4-C5-N1-C6
2	A	401	CHT	C4-C5-N1-C7
7	D	403	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
2	G	401	CHT	O6-C4-C5-N1
6	D	402	EDO	O1-C1-C2-O2
2	A	401	CHT	C4-C5-N1-C8
2	D	401	CHT	C4-C5-N1-C7
2	D	401	CHT	O6-C4-C5-N1

There are no ring outliers.

10 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	401	CHT	1	0
4	E	401	EPE	1	0
4	F	402	EPE	1	0
3	H	401	ACT	4	0
5	D	405	GOL	1	0
6	D	402	EDO	4	0
5	C	402	GOL	1	0
2	D	401	CHT	6	0
2	A	401	CHT	6	0
7	D	403	PEG	8	0

## 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	313/328 (95%)	0.03	11 (3%)	47 53	12, 19, 42, 77	0
1	B	313/328 (95%)	-0.04	12 (3%)	44 50	11, 18, 38, 80	1 (0%)
1	C	311/328 (94%)	-0.03	6 (1%)	66 73	12, 19, 38, 64	0
1	D	304/328 (92%)	-0.09	10 (3%)	49 55	11, 18, 39, 75	0
1	E	308/328 (93%)	-0.09	10 (3%)	50 57	11, 17, 40, 74	0
1	F	309/328 (94%)	0.02	12 (3%)	43 49	11, 18, 40, 75	0
1	G	312/328 (95%)	0.11	11 (3%)	47 53	12, 20, 40, 83	0
1	H	314/328 (95%)	0.09	10 (3%)	50 57	9, 20, 39, 81	1 (0%)
All	All	2484/2624 (94%)	-0.00	82 (3%)	49 55	9, 19, 40, 83	2 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	101	PHE	6.9
1	H	227	TRP	6.8
1	E	227	TRP	6.6
1	B	99	VAL	6.3
1	B	227	TRP	6.0
1	A	227	TRP	5.7
1	A	101	PHE	5.3
1	G	325	SER	5.2
1	H	228	PRO	5.1
1	F	101	PHE	5.0
1	B	325	SER	4.9
1	G	99	VAL	4.4
1	C	325	SER	4.0
1	G	205	GLY	4.0
1	H	101	PHE	3.9
1	D	325	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	F	325	SER	3.8
1	C	103	ARG	3.8
1	F	227	TRP	3.8
1	E	325	SER	3.7
1	H	325	SER	3.7
1	E	121	MET	3.6
1	E	94	GLN	3.6
1	D	226	PHE	3.5
1	C	99	VAL	3.4
1	G	101	PHE	3.3
1	D	94	GLN	3.2
1	F	228	PRO	3.1
1	D	103	ARG	3.0
1	E	119	GLN	3.0
1	B	226	PHE	3.0
1	F	94	GLN	2.9
1	A	325	SER	2.9
1	B	95	THR	2.9
1	B	228	PRO	2.9
1	C	195	LYS	2.9
1	F	160	ASP	2.8
1	H	160	ASP	2.8
1	B	323	GLY	2.8
1	H	8	ASN	2.8
1	E	205	GLY	2.7
1	G	323	GLY	2.7
1	B	98	GLU	2.7
1	G	94	GLN	2.7
1	E	103	ARG	2.7
1	F	103	ARG	2.7
1	G	206	ALA	2.7
1	B	324	TYR	2.7
1	B	8	ASN	2.7
1	D	225	PRO	2.6
1	E	88	SER	2.6
1	A	94	GLN	2.6
1	C	227	TRP	2.6
1	F	100	GLN	2.6
1	A	295	ILE	2.6
1	H	100	GLN	2.5
1	H	99	VAL	2.5
1	D	205	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	99	VAL	2.5
1	D	8	ASN	2.4
1	F	102	ARG	2.4
1	D	295	ILE	2.4
1	A	226	PHE	2.4
1	G	204	LYS	2.4
1	E	195	LYS	2.3
1	F	225	PRO	2.3
1	A	100	GLN	2.3
1	G	324	TYR	2.2
1	H	95	THR	2.2
1	D	93	ASP	2.2
1	B	205	GLY	2.2
1	E	101	PHE	2.1
1	G	226	PHE	2.1
1	F	324	TYR	2.1
1	C	204	LYS	2.1
1	D	160	ASP	2.1
1	G	95	THR	2.1
1	A	160	ASP	2.1
1	H	9	ILE	2.1
1	A	8	ASN	2.0
1	F	8	ASN	2.0
1	A	9	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 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, 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	ACT	H	401	4/4	0.74	0.22	36,37,59,71	0
2	CHT	G	401	7/7	0.75	0.18	26,28,36,38	0
4	EPE	F	402	15/15	0.78	0.20	29,58,91,116	0
3	ACT	A	402	4/4	0.80	0.14	31,38,39,43	0
4	EPE	F	401	15/15	0.83	0.16	33,55,62,64	0
5	GOL	C	402	6/6	0.83	0.19	24,41,45,49	0
2	CHT	A	401	7/7	0.85	0.15	21,30,36,52	0
7	PEG	D	403	7/7	0.85	0.15	26,44,50,50	0
7	PEG	D	404	7/7	0.85	0.17	50,52,60,67	0
4	EPE	E	401	15/15	0.86	0.15	25,46,56,57	0
2	CHT	D	401	7/7	0.89	0.13	20,27,35,41	0
5	GOL	D	405	6/6	0.89	0.12	25,43,44,44	0
4	EPE	C	401	15/15	0.91	0.12	29,38,48,48	0
6	EDO	D	402	4/4	0.91	0.10	32,38,42,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.