



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:37 AM UTC

PDB ID : 8ASA / pdb_00008asa
Title : Crystal structure of AO75L
Authors : Laugeri, M.E.; Speciale, I.; Gimeno, A.; Lin, S.; Poveda, A.; Lowary, T.; Van Etten, J.L.; Barbero, J.J.; De Castro, C.; Tonetti, M.; Rojas, A.L.
Deposited on : 2022-08-18
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 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

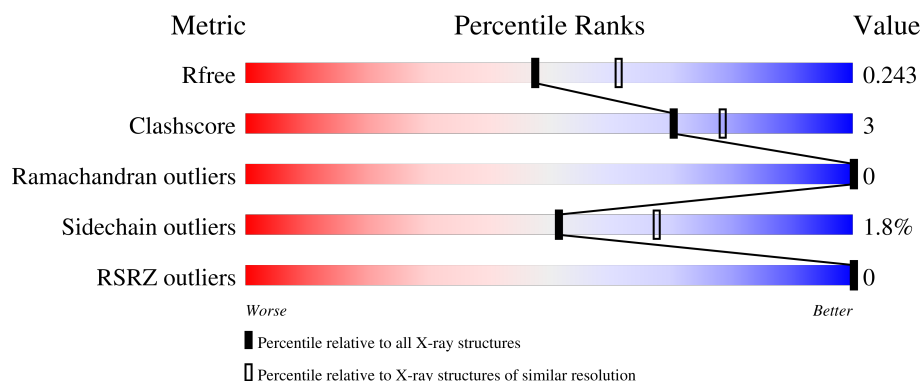
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	285	 89% 8% ..
1	B	285	 91% 8% ..
1	C	285	 90% 8% .
1	D	285	 88% 9% ..
1	E	285	 91% 8% .

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Mol	Chain	Length	Quality of chain
1	F	285	 87% 9% ..
1	G	285	 92% 6% ..
1	H	285	 88% 8% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20366 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 Exostosin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	Se	0	3	0
			2366	1524	393	439	5	5			
1	B	282	Total	C	N	O	S	Se	0	1	0
			2368	1525	395	439	4	5			
1	C	281	Total	C	N	O	S	Se	0	1	0
			2354	1516	391	438	4	5			
1	D	281	Total	C	N	O	S	Se	0	1	0
			2363	1521	394	439	4	5			
1	E	281	Total	C	N	O	S	Se	0	1	0
			2357	1517	391	440	4	5			
1	F	280	Total	C	N	O	S	Se	0	2	0
			2359	1520	390	440	4	5			
1	G	281	Total	C	N	O	S	Se	0	2	0
			2361	1520	391	441	4	5			
1	H	278	Total	C	N	O	S	Se	0	2	0
			2341	1506	389	437	4	5			

There are 40 discrepancies between the modelled and reference sequences:

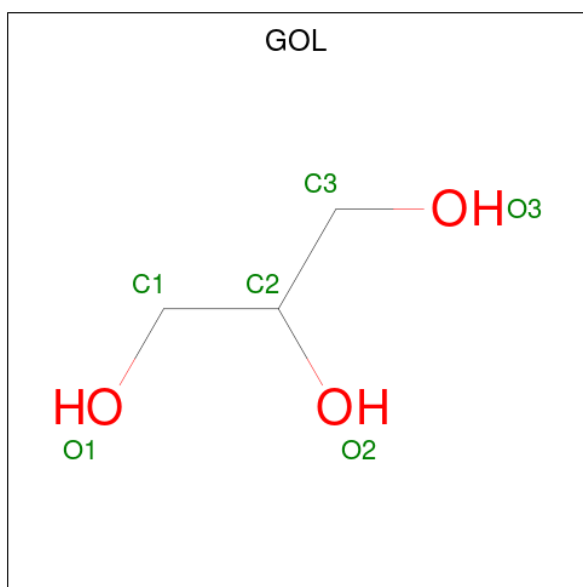
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q89410
A	-3	PRO	-	expression tag	UNP Q89410
A	-2	LEU	-	expression tag	UNP Q89410
A	-1	GLY	-	expression tag	UNP Q89410
A	0	SER	-	expression tag	UNP Q89410
B	-4	GLY	-	expression tag	UNP Q89410
B	-3	PRO	-	expression tag	UNP Q89410
B	-2	LEU	-	expression tag	UNP Q89410
B	-1	GLY	-	expression tag	UNP Q89410
B	0	SER	-	expression tag	UNP Q89410
C	-4	GLY	-	expression tag	UNP Q89410
C	-3	PRO	-	expression tag	UNP Q89410
C	-2	LEU	-	expression tag	UNP Q89410

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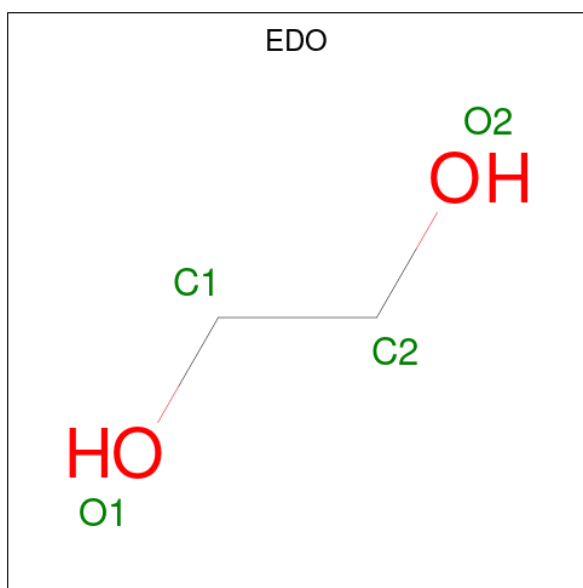
Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP Q89410
C	0	SER	-	expression tag	UNP Q89410
D	-4	GLY	-	expression tag	UNP Q89410
D	-3	PRO	-	expression tag	UNP Q89410
D	-2	LEU	-	expression tag	UNP Q89410
D	-1	GLY	-	expression tag	UNP Q89410
D	0	SER	-	expression tag	UNP Q89410
E	-4	GLY	-	expression tag	UNP Q89410
E	-3	PRO	-	expression tag	UNP Q89410
E	-2	LEU	-	expression tag	UNP Q89410
E	-1	GLY	-	expression tag	UNP Q89410
E	0	SER	-	expression tag	UNP Q89410
F	-4	GLY	-	expression tag	UNP Q89410
F	-3	PRO	-	expression tag	UNP Q89410
F	-2	LEU	-	expression tag	UNP Q89410
F	-1	GLY	-	expression tag	UNP Q89410
F	0	SER	-	expression tag	UNP Q89410
G	-4	GLY	-	expression tag	UNP Q89410
G	-3	PRO	-	expression tag	UNP Q89410
G	-2	LEU	-	expression tag	UNP Q89410
G	-1	GLY	-	expression tag	UNP Q89410
G	0	SER	-	expression tag	UNP Q89410
H	-4	GLY	-	expression tag	UNP Q89410
H	-3	PRO	-	expression tag	UNP Q89410
H	-2	LEU	-	expression tag	UNP Q89410
H	-1	GLY	-	expression tag	UNP Q89410
H	0	SER	-	expression tag	UNP Q89410

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	6	Total Mg 6 6	0	0
4	B	3	Total Mg 3 3	0	0

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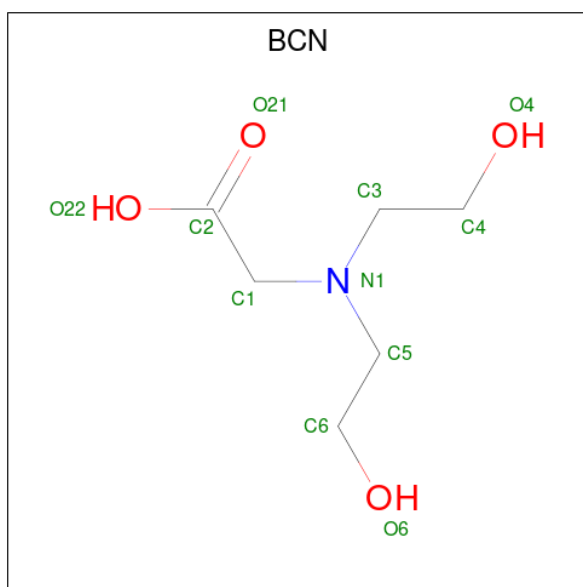
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	5	Total 5	Mg 5	0	0
4	E	3	Total 3	Mg 3	0	0
4	F	3	Total 3	Mg 3	0	0
4	G	5	Total 5	Mg 5	0	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total 2	Ca 2	0	0
5	B	3	Total 3	Ca 3	0	0
5	C	3	Total 3	Ca 3	0	0
5	D	7	Total 7	Ca 7	0	0
5	E	4	Total 4	Ca 4	0	0
5	F	2	Total 2	Ca 2	0	0
5	G	1	Total 1	Ca 1	0	0
5	H	4	Total 4	Ca 4	0	0

- Molecule 6 is BICINE (CCD ID: BCN) (formula: C₆H₁₃NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			11	6	1	4		
6	B	1	Total	C	N	O	0	0
			11	6	1	4		
6	C	1	Total	C	N	O	0	0
			11	6	1	4		
6	D	1	Total	C	N	O	0	0
			11	6	1	4		
6	D	1	Total	C	N	O	0	0
			11	6	1	4		
6	E	1	Total	C	N	O	0	0
			11	6	1	4		
6	F	1	Total	C	N	O	0	0
			11	6	1	4		
6	G	1	Total	C	N	O	0	0
			11	6	1	4		
6	H	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	151	Total	O	0	0
			151	151		
7	B	148	Total	O	0	0
			148	148		
7	C	134	Total	O	0	0
			134	134		

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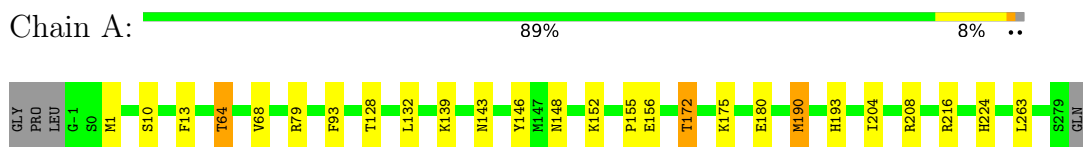
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	165	Total 165	O 165	0	0
7	E	123	Total 123	O 123	0	0
7	F	168	Total 168	O 168	0	0
7	G	148	Total 148	O 148	0	0
7	H	106	Total 106	O 106	0	0

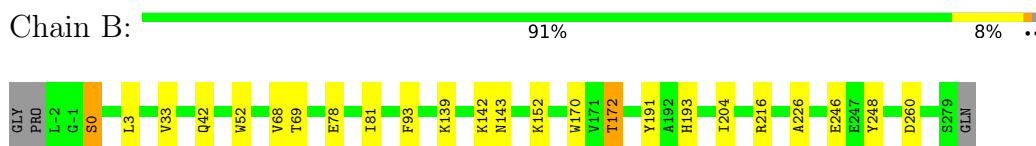
3 Residue-property plots [i](#)

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.

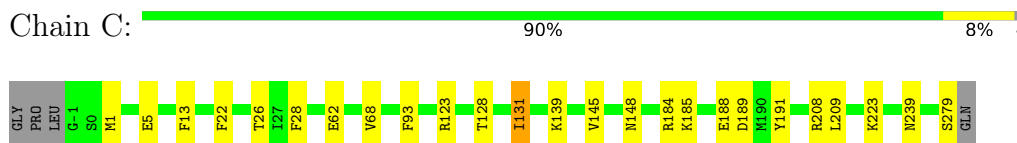
- Molecule 1: Exostosin



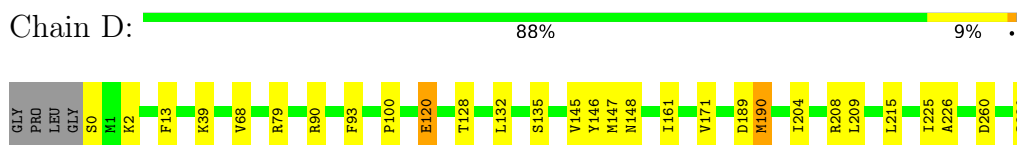
- Molecule 1: Exostosin



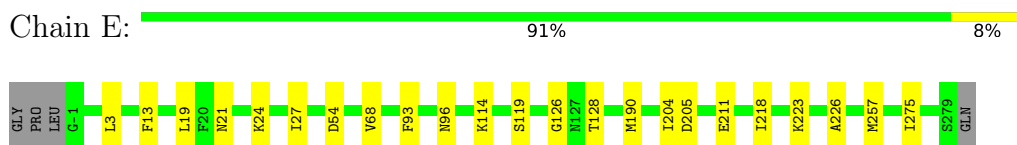
- Molecule 1: Exostosin



- Molecule 1: Exostosin

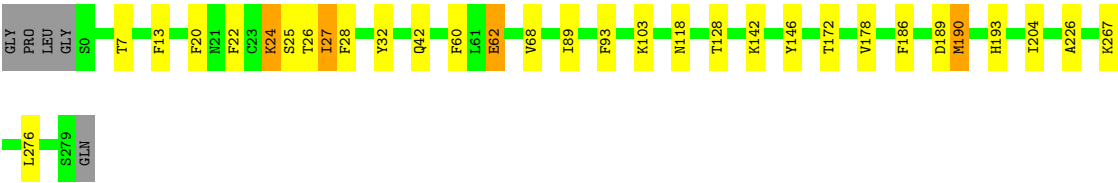


- Molecule 1: Exostosin

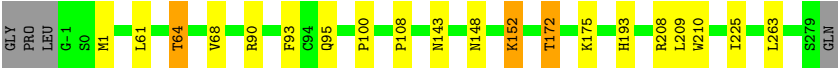
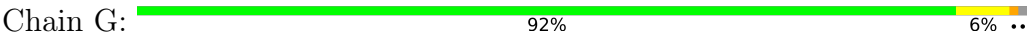


- Molecule 1: Exostosin

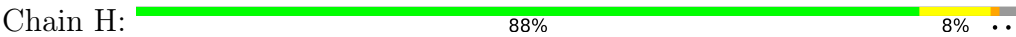




● Molecule 1: Exostosin



● Molecule 1: Exostosin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	86.71Å 90.77Å 91.68Å 90.46° 108.60° 109.71°	Depositor
Resolution (Å)	76.84 – 2.20 76.84 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.2 (76.84-2.20) 91.8 (76.84-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.194 , 0.241 0.200 , 0.243	Depositor DCC
R_{free} test set	6319 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.188 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	20366	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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: MG, CA, EDO, GOL, BCN

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	0.94	0/2426	1.34	2/3276 (0.1%)
1	B	0.95	0/2422	1.33	0/3271
1	C	0.95	0/2411	1.34	2/3257 (0.1%)
1	D	0.94	0/2420	1.32	0/3267
1	E	0.96	0/2411	1.34	0/3257
1	F	0.95	0/2416	1.32	0/3264
1	G	0.94	0/2418	1.33	1/3267 (0.0%)
1	H	0.95	0/2396	1.33	0/3234
All	All	0.95	0/19320	1.33	5/26093 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	123	ARG	CA-C-N	5.42	127.47	120.70
1	C	123	ARG	C-N-CA	5.42	127.47	120.70
1	A	155	PRO	N-CA-C	5.30	120.89	113.53
1	G	95	GLN	CB-CA-C	5.04	118.14	109.51
1	A	64	THR	CB-CA-C	5.04	115.94	110.15

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	2366	0	2335	13	0
1	B	2368	0	2335	15	0
1	C	2354	0	2318	14	0
1	D	2363	0	2330	22	0
1	E	2357	0	2315	11	0
1	F	2359	0	2317	22	0
1	G	2361	0	2322	13	0
1	H	2341	0	2306	20	0
2	A	24	0	32	0	0
2	B	18	0	24	1	0
2	C	18	0	24	0	0
2	D	6	0	8	0	0
2	F	6	0	8	0	0
2	G	6	0	8	0	0
2	H	6	0	8	0	0
3	A	16	0	24	0	0
3	B	12	0	18	0	0
3	C	16	0	24	0	0
3	D	24	0	36	1	0
3	E	12	0	18	0	0
3	F	16	0	24	0	0
3	G	16	0	24	0	0
3	H	8	0	12	0	0
4	A	6	0	0	0	0
4	B	3	0	0	0	0
4	D	5	0	0	0	0
4	E	3	0	0	0	0
4	F	3	0	0	0	0
4	G	5	0	0	0	0
5	A	2	0	0	0	0
5	B	3	0	0	0	0
5	C	3	0	0	0	0
5	D	7	0	0	0	0
5	E	4	0	0	0	0
5	F	2	0	0	0	0
5	G	1	0	0	0	0
5	H	4	0	0	0	0
6	A	11	0	11	1	0
6	B	11	0	10	0	0
6	C	11	0	11	2	0
6	D	22	0	21	1	0
6	E	11	0	10	0	0
6	F	11	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	11	0	11	0	0
6	H	11	0	10	0	0
7	A	151	0	0	0	0
7	B	148	0	0	1	0
7	C	134	0	0	0	0
7	D	165	0	0	0	0
7	E	123	0	0	1	0
7	F	168	0	0	1	0
7	G	148	0	0	1	0
7	H	106	0	0	1	0
All	All	20366	0	18964	131	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.

The worst 5 of 131 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:C:13:PHE:CE1	1:C:131:ILE:HD11	2.20	0.76
1:A:190:MSE:HE1	1:A:208:ARG:HD2	1.70	0.73
1:E:3:LEU:HD23	1:E:257:MSE:HE1	1.73	0.70
1:C:128:THR:HA	1:C:131:ILE:HD13	1.74	0.69
1:C:223:LYS:HE2	1:C:239:ASN:OD1	1.94	0.68

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	282/285 (99%)	276 (98%)	6 (2%)	0	100	100
1	B	281/285 (99%)	275 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	280/285 (98%)	268 (96%)	12 (4%)	0	100	100
1	D	280/285 (98%)	273 (98%)	7 (2%)	0	100	100
1	E	280/285 (98%)	269 (96%)	11 (4%)	0	100	100
1	F	280/285 (98%)	273 (98%)	7 (2%)	0	100	100
1	G	281/285 (99%)	275 (98%)	6 (2%)	0	100	100
1	H	276/285 (97%)	267 (97%)	9 (3%)	0	100	100
All	All	2240/2280 (98%)	2176 (97%)	64 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	266/261 (102%)	258 (97%)	8 (3%)	36	49
1	B	265/261 (102%)	261 (98%)	4 (2%)	57	73
1	C	264/261 (101%)	259 (98%)	5 (2%)	50	66
1	D	265/261 (102%)	263 (99%)	2 (1%)	73	85
1	E	264/261 (101%)	261 (99%)	3 (1%)	65	79
1	F	264/261 (101%)	256 (97%)	8 (3%)	36	49
1	G	265/261 (102%)	260 (98%)	5 (2%)	50	66
1	H	263/261 (101%)	258 (98%)	5 (2%)	50	66
All	All	2116/2088 (101%)	2076 (98%)	40 (2%)	51	66

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	142	LYS
1	H	2	LYS
1	F	190	MSE
1	G	152	LYS

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Mol	Chain	Res	Type
1	H	156[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	243	ASN
1	H	252	GLN
1	E	96	ASN
1	E	243	ASN
1	E	252	GLN

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 104 ligands modelled in this entry, 51 are monoatomic - leaving 53 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EDO	B	304	-	3,3,3	0.08	0	2,2,2	0.21	0
2	GOL	D	301	-	5,5,5	0.10	0	5,5,5	0.25	0
3	EDO	H	302	-	3,3,3	0.07	0	2,2,2	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	F	303	-	3,3,3	0.06	0	2,2,2	0.09	0
6	BCN	G	312	5	10,10,10	0.67	0	11,11,11	0.62	0
3	EDO	E	301	-	3,3,3	0.07	0	2,2,2	0.10	0
2	GOL	H	301	-	5,5,5	0.07	0	5,5,5	0.24	0
6	BCN	E	311	5	10,10,10	0.59	0	11,11,11	0.68	0
3	EDO	B	306	-	3,3,3	0.08	0	2,2,2	0.17	0
3	EDO	G	303	-	3,3,3	0.11	0	2,2,2	0.15	0
3	EDO	E	302	-	3,3,3	0.04	0	2,2,2	0.05	0
3	EDO	A	306	-	3,3,3	0.05	0	2,2,2	0.11	0
3	EDO	G	302	-	3,3,3	0.07	0	2,2,2	0.09	0
3	EDO	C	305	-	3,3,3	0.10	0	2,2,2	0.18	0
3	EDO	F	305	-	3,3,3	0.08	0	2,2,2	0.07	0
3	EDO	G	304	-	3,3,3	0.05	0	2,2,2	0.07	0
2	GOL	A	303	-	5,5,5	0.07	0	5,5,5	0.24	0
3	EDO	C	304	-	3,3,3	0.07	0	2,2,2	0.17	0
2	GOL	B	301	-	5,5,5	0.09	0	5,5,5	0.24	0
3	EDO	G	305	-	3,3,3	0.05	0	2,2,2	0.17	0
3	EDO	D	305	-	3,3,3	0.08	0	2,2,2	0.09	0
3	EDO	D	303	-	3,3,3	0.07	0	2,2,2	0.06	0
3	EDO	D	302	-	3,3,3	0.06	0	2,2,2	0.17	0
2	GOL	C	303	-	5,5,5	0.08	0	5,5,5	0.24	0
2	GOL	B	302	-	5,5,5	0.09	0	5,5,5	0.25	0
2	GOL	C	301	-	5,5,5	0.07	0	5,5,5	0.21	0
2	GOL	A	304	-	5,5,5	0.09	0	5,5,5	0.27	0
2	GOL	F	301	-	5,5,5	0.06	0	5,5,5	0.23	0
3	EDO	C	307	-	3,3,3	0.08	0	2,2,2	0.10	0
3	EDO	H	303	-	3,3,3	0.10	0	2,2,2	0.04	0
3	EDO	F	302	-	3,3,3	0.14	0	2,2,2	0.24	0
2	GOL	G	301	-	5,5,5	0.10	0	5,5,5	0.32	0
3	EDO	A	308	-	3,3,3	0.06	0	2,2,2	0.07	0
3	EDO	C	306	-	3,3,3	0.10	0	2,2,2	0.13	0
3	EDO	F	304	-	3,3,3	0.08	0	2,2,2	0.04	0
3	EDO	E	303	-	3,3,3	0.06	0	2,2,2	0.11	0
2	GOL	C	302	-	5,5,5	0.08	0	5,5,5	0.26	0
6	BCN	B	313	5	10,10,10	0.73	0	11,11,11	0.55	0
6	BCN	D	320	5	10,10,10	0.68	0	11,11,11	0.67	0
6	BCN	C	311	5	10,10,10	0.72	0	11,11,11	1.63	2 (18%)
6	BCN	F	311	5	10,10,10	0.63	0	11,11,11	0.66	0
3	EDO	A	307	-	3,3,3	0.11	0	2,2,2	0.22	0
6	BCN	A	317	5	10,10,10	0.62	0	11,11,11	0.60	0
6	BCN	D	321	5	10,10,10	0.70	0	11,11,11	0.70	0
6	BCN	H	308	5	10,10,10	0.70	0	11,11,11	0.58	0
2	GOL	A	302	4	5,5,5	0.09	0	5,5,5	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	D	306	-	3,3,3	0.04	0	2,2,2	0.08	0
3	EDO	D	307	-	3,3,3	0.11	0	2,2,2	0.32	0
2	GOL	A	301	-	5,5,5	0.10	0	5,5,5	0.29	0
3	EDO	B	305	-	3,3,3	0.09	0	2,2,2	0.25	0
3	EDO	D	304	-	3,3,3	0.09	0	2,2,2	0.08	0
2	GOL	B	303	-	5,5,5	0.10	0	5,5,5	0.28	0
3	EDO	A	305	-	3,3,3	0.08	0	2,2,2	0.14	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	304	-	-	1/1/1/1	-
2	GOL	D	301	-	-	2/4/4/4	-
3	EDO	H	302	-	-	1/1/1/1	-
3	EDO	F	303	-	-	1/1/1/1	-
6	BCN	G	312	5	-	0/10/10/10	-
3	EDO	E	301	-	-	1/1/1/1	-
2	GOL	H	301	-	-	2/4/4/4	-
6	BCN	E	311	5	-	0/10/10/10	-
3	EDO	B	306	-	-	1/1/1/1	-
3	EDO	G	303	-	-	0/1/1/1	-
3	EDO	E	302	-	-	0/1/1/1	-
3	EDO	A	306	-	-	1/1/1/1	-
3	EDO	G	302	-	-	0/1/1/1	-
3	EDO	C	305	-	-	1/1/1/1	-
3	EDO	F	305	-	-	0/1/1/1	-
3	EDO	G	304	-	-	1/1/1/1	-
2	GOL	A	303	-	-	0/4/4/4	-
3	EDO	C	304	-	-	1/1/1/1	-
2	GOL	B	301	-	-	2/4/4/4	-
3	EDO	G	305	-	-	1/1/1/1	-
3	EDO	D	305	-	-	0/1/1/1	-
3	EDO	D	303	-	-	0/1/1/1	-
3	EDO	D	302	-	-	1/1/1/1	-
2	GOL	C	303	-	-	0/4/4/4	-
2	GOL	B	302	-	-	2/4/4/4	-
2	GOL	C	301	-	-	1/4/4/4	-
2	GOL	A	304	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	F	301	-	-	4/4/4/4	-
3	EDO	C	307	-	-	1/1/1/1	-
3	EDO	H	303	-	-	0/1/1/1	-
3	EDO	F	302	-	-	1/1/1/1	-
2	GOL	G	301	-	-	2/4/4/4	-
3	EDO	A	308	-	-	1/1/1/1	-
3	EDO	C	306	-	-	1/1/1/1	-
3	EDO	F	304	-	-	1/1/1/1	-
3	EDO	E	303	-	-	1/1/1/1	-
2	GOL	C	302	-	-	0/4/4/4	-
6	BCN	B	313	5	-	1/10/10/10	-
6	BCN	D	320	5	-	0/10/10/10	-
6	BCN	C	311	5	-	4/10/10/10	-
6	BCN	F	311	5	-	0/10/10/10	-
3	EDO	A	307	-	-	1/1/1/1	-
6	BCN	A	317	5	-	0/10/10/10	-
6	BCN	D	321	5	-	5/10/10/10	-
6	BCN	H	308	5	-	0/10/10/10	-
2	GOL	A	302	4	-	4/4/4/4	-
3	EDO	D	306	-	-	1/1/1/1	-
3	EDO	D	307	-	-	1/1/1/1	-
2	GOL	A	301	-	-	2/4/4/4	-
3	EDO	B	305	-	-	1/1/1/1	-
3	EDO	D	304	-	-	1/1/1/1	-
2	GOL	B	303	-	-	0/4/4/4	-
3	EDO	A	305	-	-	1/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	311	BCN	C1-N1-C3	3.78	121.03	111.91
6	C	311	BCN	C2-C1-N1	2.74	122.45	113.77

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	302	GOL	O1-C1-C2-C3
2	A	304	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	A	304	GOL	O1-C1-C2-C3
2	B	301	GOL	O1-C1-C2-O2
2	B	301	GOL	O1-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	320	BCN	1	0
6	C	311	BCN	2	0
6	A	317	BCN	1	0
3	D	307	EDO	1	0
2	B	303	GOL	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	276/285 (96%)	-1.39	0 100 100	16, 37, 59, 75	3 (1%)
1	B	277/285 (97%)	-1.40	0 100 100	18, 38, 60, 71	1 (0%)
1	C	276/285 (96%)	-1.32	0 100 100	22, 41, 67, 79	2 (0%)
1	D	276/285 (96%)	-1.44	0 100 100	24, 35, 52, 70	1 (0%)
1	E	276/285 (96%)	-1.27	0 100 100	25, 44, 71, 90	2 (0%)
1	F	275/285 (96%)	-1.36	0 100 100	17, 39, 56, 80	3 (1%)
1	G	276/285 (96%)	-1.38	0 100 100	19, 38, 56, 75	2 (0%)
1	H	273/285 (95%)	-1.23	0 100 100	16, 48, 74, 87	2 (0%)
All	All	2205/2280 (96%)	-1.35	0 100 100	16, 39, 65, 90	16 (0%)

There are no RSRZ outliers to report.

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
2	GOL	C	303	6/6	0.95	0.05	77,79,79,79	0
3	EDO	B	306	4/4	0.95	0.09	63,65,65,66	0
4	MG	E	306	1/1	0.95	0.07	67,67,67,67	0
4	MG	G	310	1/1	0.95	0.08	48,48,48,48	0
3	EDO	H	302	4/4	0.96	0.08	53,56,56,56	0
2	GOL	C	302	6/6	0.96	0.05	79,79,81,81	0
3	EDO	D	306	4/4	0.96	0.07	54,56,57,59	0
5	CA	D	319	1/1	0.96	0.05	94,94,94,94	0
3	EDO	C	304	4/4	0.97	0.10	63,63,64,64	0
3	EDO	C	305	4/4	0.97	0.07	52,55,55,55	0
3	EDO	C	306	4/4	0.97	0.05	55,57,57,58	0
3	EDO	D	304	4/4	0.97	0.09	59,59,60,60	0
2	GOL	D	301	6/6	0.97	0.05	69,73,76,78	0
3	EDO	D	307	4/4	0.97	0.07	71,73,74,75	0
3	EDO	G	302	4/4	0.97	0.08	57,57,57,59	0
3	EDO	G	304	4/4	0.97	0.05	70,71,72,75	0
3	EDO	A	305	4/4	0.97	0.09	59,60,60,62	0
4	MG	A	311	1/1	0.97	0.06	58,58,58,58	0
4	MG	A	313	1/1	0.97	0.07	69,69,69,69	0
3	EDO	B	304	4/4	0.97	0.06	55,58,59,59	0
4	MG	G	309	1/1	0.97	0.05	56,56,56,56	0
3	EDO	B	305	4/4	0.97	0.07	49,51,53,54	0
2	GOL	A	303	6/6	0.97	0.05	74,76,77,77	0
3	EDO	E	301	4/4	0.98	0.07	53,54,54,54	0
3	EDO	E	302	4/4	0.98	0.07	57,58,59,59	0
3	EDO	E	303	4/4	0.98	0.05	71,71,71,72	0
3	EDO	F	302	4/4	0.98	0.07	55,56,57,58	0
3	EDO	F	303	4/4	0.98	0.08	59,59,59,60	0
3	EDO	F	304	4/4	0.98	0.06	58,58,59,60	0
3	EDO	F	305	4/4	0.98	0.07	72,73,73,73	0
3	EDO	A	306	4/4	0.98	0.07	57,57,59,59	0
3	EDO	G	303	4/4	0.98	0.09	60,61,62,62	0
3	EDO	A	307	4/4	0.98	0.06	51,55,57,60	0
3	EDO	G	305	4/4	0.98	0.06	62,64,65,68	0
3	EDO	A	308	4/4	0.98	0.08	57,58,58,59	0
3	EDO	H	303	4/4	0.98	0.04	38,39,41,41	0
4	MG	A	310	1/1	0.98	0.05	68,68,68,68	0
3	EDO	C	307	4/4	0.98	0.05	62,63,63,63	0
4	MG	A	312	1/1	0.98	0.06	80,80,80,80	0
3	EDO	D	303	4/4	0.98	0.04	39,42,42,42	0
4	MG	B	307	1/1	0.98	0.04	63,63,63,63	0
4	MG	D	308	1/1	0.98	0.04	54,54,54,54	0
4	MG	D	309	1/1	0.98	0.09	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	D	310	1/1	0.98	0.05	57,57,57,57	0
4	MG	D	311	1/1	0.98	0.06	51,51,51,51	0
4	MG	D	312	1/1	0.98	0.06	62,62,62,62	0
4	MG	E	304	1/1	0.98	0.07	60,60,60,60	0
2	GOL	A	301	6/6	0.98	0.05	49,56,59,59	0
4	MG	F	306	1/1	0.98	0.06	61,61,61,61	0
4	MG	F	307	1/1	0.98	0.07	56,56,56,56	0
4	MG	G	307	1/1	0.98	0.04	56,56,56,56	0
4	MG	G	308	1/1	0.98	0.04	63,63,63,63	0
3	EDO	D	305	4/4	0.98	0.07	63,65,65,66	0
2	GOL	F	301	6/6	0.98	0.05	57,58,59,60	0
5	CA	A	316	1/1	0.98	0.08	61,61,61,61	0
5	CA	B	310	1/1	0.98	0.06	76,76,76,76	0
5	CA	B	312	1/1	0.98	0.06	87,87,87,87	0
5	CA	C	309	1/1	0.98	0.04	80,80,80,80	0
5	CA	D	314	1/1	0.98	0.08	73,73,73,73	0
5	CA	D	315	1/1	0.98	0.07	67,67,67,67	0
5	CA	D	317	1/1	0.98	0.04	94,94,94,94	0
2	GOL	B	302	6/6	0.98	0.06	63,69,70,71	0
5	CA	F	310	1/1	0.98	0.06	97,97,97,97	0
5	CA	H	307	1/1	0.98	0.06	76,76,76,76	0
3	EDO	D	302	4/4	0.99	0.06	54,55,57,57	0
2	GOL	B	303	6/6	0.99	0.06	52,60,62,66	0
2	GOL	G	301	6/6	0.99	0.04	59,60,60,61	0
4	MG	A	309	1/1	0.99	0.03	56,56,56,56	0
2	GOL	H	301	6/6	0.99	0.05	56,59,61,61	0
2	GOL	C	301	6/6	0.99	0.04	43,46,48,51	0
5	CA	C	310	1/1	0.99	0.05	75,75,75,75	0
5	CA	D	313	1/1	0.99	0.05	74,74,74,74	0
4	MG	E	305	1/1	0.99	0.10	68,68,68,68	0
2	GOL	A	304	6/6	0.99	0.03	44,46,47,47	0
2	GOL	B	301	6/6	0.99	0.04	47,50,51,53	0
5	CA	D	318	1/1	0.99	0.04	75,75,75,75	0
2	GOL	A	302	6/6	0.99	0.04	42,47,50,55	0
5	CA	E	309	1/1	0.99	0.03	82,82,82,82	0
5	CA	E	310	1/1	0.99	0.04	90,90,90,90	0
4	MG	B	308	1/1	0.99	0.03	31,31,31,31	0
5	CA	H	306	1/1	0.99	0.03	64,64,64,64	0
4	MG	B	309	1/1	0.99	0.03	47,47,47,47	0
6	BCN	A	317	11/11	0.99	0.03	31,33,33,34	0
6	BCN	B	313	11/11	0.99	0.03	31,32,33,34	0
6	BCN	C	311	11/11	0.99	0.03	33,34,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	BCN	D	320	11/11	0.99	0.02	25,28,30,32	0
6	BCN	D	321	11/11	0.99	0.05	50,60,67,69	0
6	BCN	E	311	11/11	0.99	0.03	30,30,33,34	0
6	BCN	F	311	11/11	0.99	0.03	30,33,37,37	0
6	BCN	G	312	11/11	0.99	0.03	26,28,29,31	0
6	BCN	H	308	11/11	0.99	0.03	32,34,35,36	0
5	CA	H	304	1/1	1.00	0.05	47,47,47,47	0
5	CA	H	305	1/1	1.00	0.02	34,34,34,34	0
5	CA	D	316	1/1	1.00	0.01	28,28,28,28	0
5	CA	C	308	1/1	1.00	0.01	33,33,33,33	0
5	CA	A	315	1/1	1.00	0.03	32,32,32,32	0
4	MG	F	308	1/1	1.00	0.03	30,30,30,30	0
5	CA	E	307	1/1	1.00	0.03	44,44,44,44	0
5	CA	E	308	1/1	1.00	0.01	36,36,36,36	0
4	MG	G	306	1/1	1.00	0.02	29,29,29,29	0
5	CA	B	311	1/1	1.00	0.02	35,35,35,35	0
5	CA	F	309	1/1	1.00	0.01	32,32,32,32	0
4	MG	A	314	1/1	1.00	0.02	31,31,31,31	0
5	CA	G	311	1/1	1.00	0.02	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.