



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:57 AM UTC

PDB ID : 3QJX / pdb_00003qjx
Title : Crystal Structure of E. coli Aminopeptidase N in complex with L-Serine
Authors : Addlagatta, A.; Gumpena, R.; Kishor, C.; Ganji, R.J.
Deposited on : 2011-01-31
Resolution : 1.45 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

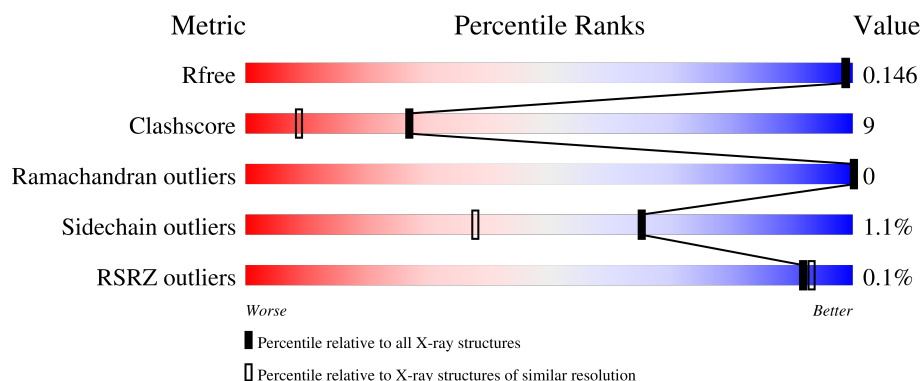
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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	891	80% 15% ..

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
5	MLI	A	950	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	A	970	-	X	-	-
6	GOL	A	972	-	X	-	-
6	GOL	A	977	-	-	X	-
6	GOL	A	978	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8314 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 Aminopeptidase N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	866	7296	4638	1253	1377	28	0	62	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP P04825
A	-19	GLY	-	expression tag	UNP P04825
A	-18	SER	-	expression tag	UNP P04825
A	-17	SER	-	expression tag	UNP P04825
A	-16	HIS	-	expression tag	UNP P04825
A	-15	HIS	-	expression tag	UNP P04825
A	-14	HIS	-	expression tag	UNP P04825
A	-13	HIS	-	expression tag	UNP P04825
A	-12	HIS	-	expression tag	UNP P04825
A	-11	HIS	-	expression tag	UNP P04825
A	-10	SER	-	expression tag	UNP P04825
A	-9	SER	-	expression tag	UNP P04825
A	-8	GLY	-	expression tag	UNP P04825
A	-7	GLU	-	expression tag	UNP P04825
A	-6	ASN	-	expression tag	UNP P04825
A	-5	LEU	-	expression tag	UNP P04825
A	-4	TYR	-	expression tag	UNP P04825
A	-3	PHE	-	expression tag	UNP P04825
A	-2	GLN	-	expression tag	UNP P04825
A	-1	GLY	-	expression tag	UNP P04825
A	0	HIS	-	expression tag	UNP P04825

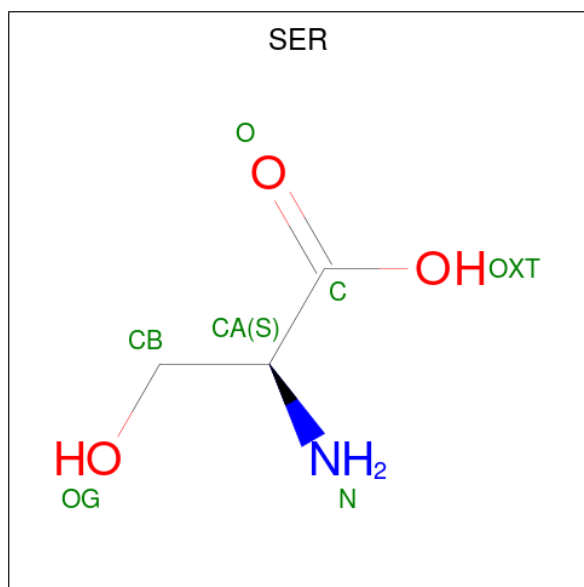
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Na	0	0
			3	3		

- Molecule 4 is SERINE (CCD ID: SER) (formula: C₃H₇NO₃).



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

- Molecule 5 is MALONATE ION (CCD ID: MLI) (formula: C₃H₂O₄).



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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

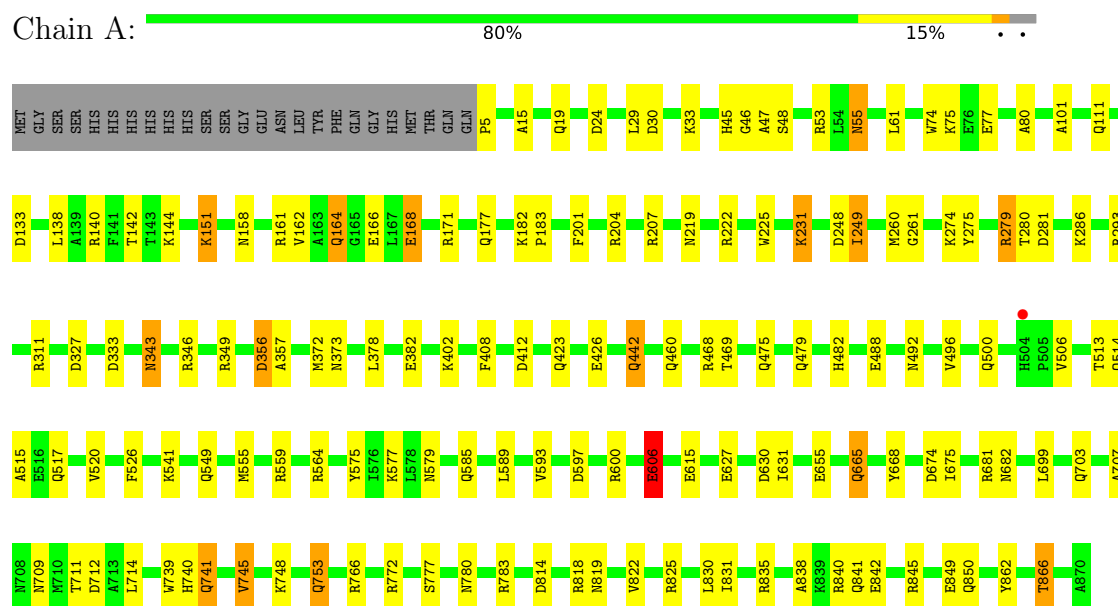
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	922	Total	O	0	0
			922	922		

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: Aminopeptidase N



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	120.23Å 120.23Å 170.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.74 – 1.45 35.74 – 1.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (35.74-1.45) 99.9 (35.74-1.45)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.120 , 0.147 0.119 , 0.146	Depositor DCC
R_{free} test set	7641 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å ²)	12.1	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	8314	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: GOL, NA, ZN, MLI

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.67	58/7629 (0.8%)	1.41	26/10345 (0.3%)

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	207	ARG	CD-NE	10.42	1.60	1.46
1	A	260	MET	N-CA	8.46	1.55	1.46
1	A	831	ILE	CA-CB	-7.83	1.45	1.54
1	A	231	LYS	CE-NZ	7.43	1.71	1.49
1	A	585	GLN	CG-CD	7.39	1.70	1.52
1	A	830	LEU	CB-CG	-7.34	1.38	1.53
1	A	29	LEU	CB-CG	-7.01	1.39	1.53
1	A	161	ARG	CB-CG	-6.90	1.31	1.52
1	A	140	ARG	CZ-NH1	6.62	1.42	1.32
1	A	343	ASN	CG-OD1	6.58	1.36	1.23
1	A	866	THR	CB-OG1	-6.57	1.33	1.43
1	A	772	ARG	CD-NE	6.45	1.55	1.46
1	A	161	ARG	CZ-NH2	6.43	1.41	1.33
1	A	161	ARG	NE-CZ	6.34	1.40	1.33
1	A	699	LEU	N-CA	6.29	1.53	1.46
1	A	144	LYS	CD-CE	-6.28	1.33	1.52
1	A	161	ARG	CZ-NH1	6.25	1.41	1.32
1	A	207	ARG	CG-CD	6.20	1.71	1.52
1	A	231	LYS	CD-CE	-6.19	1.33	1.52
1	A	549	GLN	CG-CD	6.11	1.67	1.52
1	A	475	GLN	CA-CB	6.05	1.63	1.53
1	A	681	ARG	CD-NE	6.03	1.54	1.46
1	A	506	VAL	CA-CB	6.03	1.62	1.54
1	A	168	GLU	C-O	6.00	1.32	1.23
1	A	630	ASP	C-O	5.98	1.31	1.24
1	A	161	ARG	CG-CD	5.93	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	766	ARG	CG-CD	5.93	1.70	1.52
1	A	164	GLN	CB-CG	-5.91	1.34	1.52
1	A	47	ALA	C-O	5.83	1.30	1.23
1	A	520	VAL	C-O	5.82	1.30	1.24
1	A	460	GLN	N-CA	5.80	1.52	1.46
1	A	630	ASP	N-CA	5.71	1.53	1.46
1	A	357	ALA	C-O	5.53	1.31	1.24
1	A	589	LEU	C-O	5.45	1.30	1.23
1	A	707	ALA	CA-CB	5.44	1.62	1.53
1	A	866	THR	CA-CB	-5.43	1.44	1.53
1	A	442	GLN	CD-OE1	5.43	1.33	1.23
1	A	665	GLN	N-CA	5.41	1.52	1.46
1	A	46	GLY	C-O	5.37	1.29	1.23
1	A	818	ARG	N-CA	5.37	1.52	1.46
1	A	606	GLU	CG-CD	5.37	1.65	1.52
1	A	841	GLN	CB-CG	-5.36	1.36	1.52
1	A	55	ASN	CG-OD1	5.34	1.33	1.23
1	A	593	VAL	CA-CB	5.33	1.60	1.54
1	A	15	ALA	CA-C	5.30	1.59	1.53
1	A	45	HIS	C-O	5.29	1.30	1.23
1	A	500	GLN	CA-C	-5.28	1.46	1.52
1	A	777	SER	CA-C	5.22	1.59	1.52
1	A	745	VAL	CA-C	5.21	1.59	1.52
1	A	19	GLN	C-O	5.21	1.30	1.23
1	A	225	TRP	CA-C	5.17	1.59	1.52
1	A	515	ALA	CA-C	5.13	1.59	1.52
1	A	631	ILE	CG1-CD1	5.13	1.71	1.51
1	A	482	HIS	C-N	5.11	1.37	1.33
1	A	766	ARG	CZ-NH1	5.07	1.39	1.32
1	A	577	LYS	CD-CE	-5.04	1.37	1.52
1	A	835	ARG	CZ-NH2	5.04	1.40	1.33
1	A	372	MET	CA-C	5.04	1.59	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	373	ASN	CB-CG-ND2	-8.15	104.17	116.40
1	A	681	ARG	NE-CZ-NH2	7.79	126.21	119.20
1	A	48	SER	CA-CB-OG	-7.36	96.37	111.10
1	A	356	ASP	O-C-N	7.27	132.49	122.46
1	A	426	GLU	CB-CG-CD	-6.72	101.18	112.60
1	A	279	ARG	NE-CZ-NH1	-6.56	114.94	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	866	THR	OG1-CB-CG2	-6.35	96.61	109.30
1	A	207	ARG	NE-CZ-NH1	-6.29	115.21	121.50
1	A	279	ARG	NE-CZ-NH2	6.29	124.86	119.20
1	A	357	ALA	N-CA-C	-6.07	105.45	112.92
1	A	675	ILE	CA-C-O	-6.04	114.67	120.95
1	A	469	THR	N-CA-C	-5.80	100.13	109.40
1	A	166	GLU	CA-CB-CG	-5.76	102.59	114.10
1	A	248	ASP	N-CA-CB	-5.74	102.09	110.53
1	A	333	ASP	CA-C-O	-5.44	114.65	120.42
1	A	201	PHE	CA-C-N	-5.35	115.62	123.00
1	A	201	PHE	C-N-CA	-5.35	115.62	123.00
1	A	838	ALA	N-CA-C	5.33	117.09	111.28
1	A	835	ARG	NE-CZ-NH2	5.32	123.98	119.20
1	A	373	ASN	CA-CB-CG	-5.31	107.29	112.60
1	A	402	LYS	CB-CG-CD	-5.30	99.11	111.30
1	A	311	ARG	NE-CZ-NH1	-5.21	116.29	121.50
1	A	835	ARG	NE-CZ-NH1	-5.07	116.43	121.50
1	A	549	GLN	CA-C-O	-5.05	114.17	119.97
1	A	575	TYR	CA-CB-CG	-5.05	104.81	113.90
1	A	579	ASN	CA-CB-CG	-5.04	107.56	112.60

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	7296	0	7277	134	1
2	A	1	0	0	0	0
3	A	3	0	0	0	0
4	A	7	0	4	0	0
5	A	7	0	2	0	0
6	A	78	0	76	19	0
7	A	922	0	0	37	1
All	All	8314	0	7359	136	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 9.

All (136) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:LYS:CE	1:A:231:LYS:NZ	1.71	1.48
1:A:825[B]:ARG:NH2	7:A:1776:HOH:O	1.58	1.31
1:A:627[A]:GLU:HG3	7:A:1384:HOH:O	1.23	1.27
1:A:783[B]:ARG:NH2	1:A:825[B]:ARG:HD2	1.49	1.26
1:A:783[B]:ARG:HH21	1:A:825[B]:ARG:CD	1.52	1.23
1:A:825[B]:ARG:CZ	7:A:1362:HOH:O	1.90	1.17
1:A:343:ASN:OD1	1:A:346[A]:ARG:NH1	1.76	1.16
1:A:346[A]:ARG:NH2	1:A:615:GLU:OE1	1.81	1.12
1:A:204[B]:ARG:HG3	1:A:204[B]:ARG:HH11	1.00	1.11
1:A:627[A]:GLU:HG2	7:A:1796:HOH:O	1.49	1.11
1:A:783[B]:ARG:HG2	1:A:783[B]:ARG:HH11	1.08	1.10
1:A:783[A]:ARG:NH1	6:A:977:GOL:O3	1.85	1.10
1:A:783[B]:ARG:NH2	1:A:825[B]:ARG:CD	2.11	1.09
1:A:5:PRO:N	7:A:1167:HOH:O	1.84	1.08
1:A:488[B]:GLU:OE1	1:A:559:ARG:NH2	1.86	1.06
1:A:783[B]:ARG:HH21	1:A:825[B]:ARG:HD2	0.90	1.04
1:A:825[B]:ARG:HH11	1:A:825[B]:ARG:HG3	1.23	1.01
1:A:825[B]:ARG:NH1	7:A:1362:HOH:O	1.93	0.97
1:A:346[B]:ARG:NH1	7:A:1801:HOH:O	1.98	0.96
1:A:281[A]:ASP:OD1	7:A:943:HOH:O	1.84	0.95
1:A:346[A]:ARG:NH1	7:A:1075:HOH:O	2.00	0.95
1:A:783[B]:ARG:NH2	1:A:825[B]:ARG:NE	2.15	0.95
1:A:249[A]:ILE:HG22	7:A:1526:HOH:O	1.69	0.93
1:A:249[A]:ILE:CG2	7:A:1526:HOH:O	2.15	0.93
1:A:204[B]:ARG:HH11	1:A:204[B]:ARG:CG	1.81	0.93
1:A:279:ARG:NH1	1:A:281[A]:ASP:OD1	2.03	0.92
1:A:845[B]:ARG:NH2	7:A:1666:HOH:O	2.04	0.91
1:A:627[B]:GLU:HG3	7:A:1367:HOH:O	1.68	0.91
1:A:279:ARG:NH1	1:A:281[A]:ASP:OD2	2.05	0.90
1:A:783[A]:ARG:CZ	7:A:1776:HOH:O	2.20	0.89
1:A:783[B]:ARG:HG2	1:A:783[B]:ARG:NH1	1.78	0.88
1:A:514:GLN:H	1:A:517[B]:GLN:HE22	1.17	0.88
1:A:825[B]:ARG:HG3	1:A:825[B]:ARG:NH1	1.83	0.87
1:A:279:ARG:NH1	1:A:281[A]:ASP:CG	2.34	0.85
1:A:204[B]:ARG:HG3	1:A:204[B]:ARG:NH1	1.80	0.85
1:A:783[A]:ARG:HH12	6:A:977:GOL:C3	1.90	0.83
1:A:286:LYS:HE3	6:A:978:GOL:O2	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274[A]:LYS:NZ	6:A:982:GOL:O3	2.10	0.83
1:A:541:LYS:HE2	1:A:627[B]:GLU:OE1	1.82	0.80
1:A:783[B]:ARG:NH2	1:A:825[B]:ARG:HE	1.78	0.80
1:A:231:LYS:NZ	1:A:231:LYS:CD	2.42	0.80
1:A:442:GLN:HE22	1:A:479:GLN:H	1.30	0.78
1:A:286:LYS:HE3	6:A:978:GOL:HO2	1.48	0.78
1:A:597:ASP:OD1	1:A:600[B]:ARG:NH1	2.18	0.76
1:A:842[B]:GLU:HG2	7:A:886:HOH:O	1.87	0.75
1:A:204[B]:ARG:CG	1:A:204[B]:ARG:NH1	2.44	0.75
1:A:783[A]:ARG:NE	7:A:1776:HOH:O	2.19	0.75
1:A:274[A]:LYS:HZ3	6:A:982:GOL:HO3	1.35	0.74
1:A:783[B]:ARG:HH11	1:A:783[B]:ARG:CG	1.93	0.74
1:A:24[B]:ASP:CG	7:A:1125:HOH:O	2.29	0.74
1:A:286:LYS:CE	6:A:978:GOL:O2	2.35	0.73
1:A:513:THR:H	1:A:517[A]:GLN:HE22	1.38	0.69
1:A:627[B]:GLU:OE2	7:A:1797:HOH:O	2.09	0.69
1:A:24[B]:ASP:OD1	7:A:1125:HOH:O	2.11	0.68
1:A:55:ASN:HD22	1:A:133:ASP:H	1.43	0.67
1:A:171[A]:ARG:HD3	7:A:946:HOH:O	1.95	0.65
1:A:24[B]:ASP:OD2	7:A:1125:HOH:O	2.14	0.65
1:A:783[B]:ARG:NH1	1:A:783[B]:ARG:CG	2.55	0.65
1:A:783[B]:ARG:CZ	1:A:825[B]:ARG:HE	2.12	0.63
1:A:219:ASN:ND2	1:A:222:ARG:HH21	1.99	0.61
1:A:53[B]:ARG:HH22	1:A:77[B]:GLU:CD	2.09	0.61
1:A:77[B]:GLU:HG2	1:A:80:ALA:HB3	1.83	0.60
1:A:74:TRP:HE1	6:A:972:GOL:H11	1.66	0.60
1:A:349[A]:ARG:NH2	7:A:889:HOH:O	2.07	0.59
1:A:627[A]:GLU:CG	7:A:1796:HOH:O	2.23	0.59
1:A:274[B]:LYS:HD3	7:A:1597:HOH:O	2.02	0.59
1:A:158:ASN:ND2	1:A:182[B]:LYS:HZ1	2.02	0.58
1:A:783[B]:ARG:CZ	1:A:825[B]:ARG:NE	2.67	0.58
1:A:555:MET:O	1:A:564[B]:ARG:HD3	2.04	0.57
1:A:714:LEU:HD22	1:A:748:LYS:HD3	1.85	0.57
1:A:514:GLN:H	1:A:517[B]:GLN:NE2	1.95	0.57
1:A:600[B]:ARG:HD3	1:A:655:GLU:OE2	2.05	0.56
1:A:249[A]:ILE:HG23	7:A:1526:HOH:O	1.92	0.56
1:A:783[A]:ARG:CZ	6:A:977:GOL:O3	2.52	0.56
1:A:158:ASN:CG	1:A:182[B]:LYS:HZ1	2.13	0.56
1:A:275:TYR:OH	6:A:977:GOL:H11	2.04	0.56
1:A:850:GLN:OE1	7:A:1273:HOH:O	2.18	0.56
1:A:709:ASN:ND2	1:A:712:ASP:H	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LYS:HE3	1:A:77[A]:GLU:OE2	2.06	0.55
1:A:261:GLY:HA2	6:A:977:GOL:H31	1.88	0.55
1:A:442:GLN:NE2	1:A:479:GLN:H	2.02	0.54
1:A:77[B]:GLU:CG	1:A:80:ALA:HB3	2.38	0.54
1:A:849[A]:GLU:CD	7:A:1156:HOH:O	2.52	0.53
1:A:741[A]:GLN:NE2	1:A:741[A]:GLN:H	2.08	0.52
1:A:138[B]:LEU:HD12	1:A:183:PRO:HD3	1.92	0.52
1:A:168:GLU:HG2	7:A:908:HOH:O	2.10	0.51
1:A:627[B]:GLU:CD	7:A:1797:HOH:O	2.53	0.51
1:A:849[A]:GLU:OE1	7:A:1156:HOH:O	2.19	0.51
1:A:753:GLN:HE21	1:A:753:GLN:HA	1.76	0.51
1:A:142[B]:THR:HG23	1:A:177[B]:GLN:HG2	1.93	0.50
1:A:492:ASN:HB3	1:A:526:PHE:CE2	2.47	0.50
1:A:783[A]:ARG:HH12	6:A:977:GOL:H32	1.73	0.50
1:A:682:ASN:ND2	1:A:703:GLN:HE22	2.10	0.49
1:A:274[A]:LYS:NZ	6:A:977:GOL:H32	2.29	0.48
1:A:423[B]:GLN:NE2	7:A:902:HOH:O	2.36	0.47
1:A:249[A]:ILE:HD11	7:A:1519:HOH:O	2.14	0.47
1:A:665:GLN:HE22	1:A:674:ASP:HA	1.80	0.47
1:A:343:ASN:OD1	1:A:346[B]:ARG:HD2	2.14	0.47
1:A:468[B]:ARG:HG3	1:A:468[B]:ARG:HH11	1.80	0.47
1:A:488[B]:GLU:HG3	1:A:496:VAL:HG13	1.97	0.47
1:A:709:ASN:HD21	1:A:712:ASP:H	1.61	0.47
1:A:279:ARG:HG3	1:A:281[A]:ASP:OD1	2.15	0.46
1:A:682:ASN:HD21	1:A:703:GLN:HE22	1.64	0.46
1:A:101:ALA:HA	1:A:111[B]:GLN:OE1	2.15	0.46
1:A:862:TYR:O	1:A:866:THR:HG23	2.16	0.46
1:A:74:TRP:NE1	6:A:972:GOL:H11	2.32	0.45
1:A:606:GLU:CD	1:A:606:GLU:H	2.23	0.45
1:A:825[A]:ARG:NH1	7:A:885:HOH:O	2.50	0.45
1:A:61:LEU:O	6:A:973:GOL:H31	2.17	0.45
1:A:378:LEU:O	1:A:382[B]:GLU:HB2	2.18	0.44
1:A:53[B]:ARG:HG3	1:A:53[B]:ARG:NH1	2.33	0.44
1:A:158:ASN:CG	1:A:182[B]:LYS:NZ	2.74	0.44
1:A:151:LYS:HB2	1:A:151:LYS:HE2	1.47	0.44
1:A:293[B]:ARG:NH1	7:A:1636:HOH:O	2.48	0.44
1:A:274[B]:LYS:HE3	1:A:274[B]:LYS:HB3	1.58	0.43
1:A:468[B]:ARG:HG3	1:A:468[B]:ARG:NH1	2.34	0.43
1:A:739:TRP:CG	1:A:745:VAL:HG11	2.53	0.43
1:A:30:ASP:HB3	1:A:33:LYS:O	2.19	0.43
1:A:274[B]:LYS:HE3	1:A:780[B]:ASN:HD21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:972:GOL:H32	7:A:1515:HOH:O	2.18	0.43
1:A:408:PHE:O	1:A:412[A]:ASP:HB2	2.18	0.43
1:A:840:ARG:HG2	7:A:934:HOH:O	2.18	0.42
1:A:814:ASP:OD1	1:A:814:ASP:C	2.62	0.42
1:A:53[B]:ARG:HG3	1:A:53[B]:ARG:HH11	1.85	0.42
1:A:75:LYS:HE3	1:A:77[A]:GLU:CD	2.45	0.41
1:A:819:ASN:HB3	1:A:822[B]:VAL:HG22	2.03	0.41
6:A:976:GOL:H31	7:A:1467:HOH:O	2.19	0.41
1:A:162:VAL:HG21	1:A:177[B]:GLN:HG3	2.03	0.41
1:A:274[A]:LYS:HZ3	6:A:977:GOL:H32	1.85	0.41
1:A:740:HIS:CE1	1:A:741[B]:GLN:HG3	2.56	0.40
1:A:279:ARG:HH12	1:A:281[A]:ASP:CG	2.09	0.40
1:A:709:ASN:HD22	1:A:711:THR:H	1.69	0.40
1:A:274[A]:LYS:NZ	6:A:982:GOL:HO3	2.06	0.40
1:A:280[B]:THR:HG23	1:A:668:TYR:CD2	2.56	0.40
1:A:488[B]:GLU:OE1	1:A:559:ARG:CZ	2.64	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:A:204[B]:ARG:NE	7:A:963:HOH:O[4_565]	2.17	0.03

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	926/891 (104%)	912 (98%)	14 (2%)	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	802/763 (105%)	792 (99%)	10 (1%)	63 33

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	LYS
1	A	164	GLN
1	A	249[A]	ILE
1	A	249[B]	ILE
1	A	327	ASP
1	A	356	ASP
1	A	606	GLU
1	A	741[A]	GLN
1	A	741[B]	GLN
1	A	753	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	55	ASN
1	A	219	ASN
1	A	340	ASN
1	A	442	GLN
1	A	514	GLN
1	A	623	ASN
1	A	663	ASN
1	A	665	GLN
1	A	682	ASN
1	A	709	ASN
1	A	753	GLN
1	A	770	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 4 are monoatomic - leaving 15 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	$\# Z > 2$
6	GOL	A	979	-	5,5,5	1.00	0	5,5,5	1.89	2 (40%)
6	GOL	A	972	-	5,5,5	3.19	3 (60%)	5,5,5	2.49	2 (40%)
6	GOL	A	974	-	5,5,5	1.74	2 (40%)	5,5,5	1.39	1 (20%)
6	GOL	A	975	-	5,5,5	1.28	0	5,5,5	1.47	2 (40%)
6	GOL	A	982	-	5,5,5	0.92	0	5,5,5	1.80	1 (20%)
6	GOL	A	978	-	5,5,5	1.29	0	5,5,5	2.42	3 (60%)
4	SER	A	900	2	4,6,6	1.26	1 (25%)	2,7,7	0.65	0
6	GOL	A	973	-	5,5,5	1.02	0	5,5,5	1.66	1 (20%)
6	GOL	A	970	-	5,5,5	2.29	2 (40%)	5,5,5	2.40	3 (60%)
5	MLI	A	950	-	6,6,6	2.01	3 (50%)	7,7,7	3.17	4 (57%)
6	GOL	A	981	-	5,5,5	0.59	0	5,5,5	1.61	1 (20%)
6	GOL	A	976	-	5,5,5	1.27	1 (20%)	5,5,5	1.87	1 (20%)
6	GOL	A	977	-	5,5,5	0.76	0	5,5,5	2.36	2 (40%)
6	GOL	A	983	-	5,5,5	0.98	0	5,5,5	1.20	0
6	GOL	A	971	-	5,5,5	0.83	0	5,5,5	0.92	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
6	GOL	A	979	-	-	3/4/4/4	-
6	GOL	A	972	-	-	3/4/4/4	-
6	GOL	A	974	-	-	0/4/4/4	-
6	GOL	A	975	-	-	1/4/4/4	-
6	GOL	A	982	-	-	2/4/4/4	-
6	GOL	A	978	-	-	3/4/4/4	-
4	SER	A	900	2	-	0/6/6/6	-
6	GOL	A	973	-	-	4/4/4/4	-
6	GOL	A	970	-	-	2/4/4/4	-
5	MLI	A	950	-	-	1/4/4/4	-
6	GOL	A	981	-	-	3/4/4/4	-
6	GOL	A	976	-	-	2/4/4/4	-
6	GOL	A	977	-	-	2/4/4/4	-
6	GOL	A	983	-	-	2/4/4/4	-
6	GOL	A	971	-	-	0/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	972	GOL	O2-C2	-5.34	1.27	1.43
6	A	972	GOL	C3-C2	3.72	1.66	1.51
6	A	970	GOL	O2-C2	3.27	1.52	1.43
5	A	950	MLI	C1-C2	3.03	1.55	1.51
5	A	950	MLI	C1-C3	3.02	1.55	1.51
6	A	970	GOL	C1-C2	2.91	1.62	1.51
6	A	972	GOL	O3-C3	2.88	1.54	1.42
6	A	976	GOL	O2-C2	-2.68	1.35	1.43
6	A	974	GOL	O2-C2	-2.31	1.36	1.43
6	A	974	GOL	C1-C2	2.26	1.60	1.51
5	A	950	MLI	O6-C2	2.22	1.29	1.22
4	A	900	SER	O-C	2.12	1.28	1.22

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	950	MLI	O6-C2-C1	-5.60	106.17	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	972	GOL	O1-C1-C2	-4.36	90.73	110.38
6	A	970	GOL	C3-C2-C1	-4.01	97.08	111.80
6	A	978	GOL	O2-C2-C1	-3.87	93.14	109.18
6	A	977	GOL	O2-C2-C1	3.81	124.96	109.18
5	A	950	MLI	O7-C2-C1	3.69	125.94	114.51
6	A	982	GOL	O2-C2-C3	3.48	123.60	109.18
6	A	972	GOL	O2-C2-C3	3.41	123.29	109.18
5	A	950	MLI	O8-C3-C1	-3.08	113.34	122.11
6	A	976	GOL	O2-C2-C3	-3.05	96.55	109.18
5	A	950	MLI	C3-C1-C2	-2.96	102.51	112.95
6	A	981	GOL	O2-C2-C1	2.91	121.25	109.18
6	A	973	GOL	C3-C2-C1	2.88	122.38	111.80
6	A	978	GOL	O3-C3-C2	2.80	122.97	110.38
6	A	979	GOL	O3-C3-C2	2.64	122.26	110.38
6	A	974	GOL	O1-C1-C2	2.61	122.12	110.38
6	A	979	GOL	O2-C2-C1	-2.54	98.65	109.18
6	A	977	GOL	O2-C2-C3	2.47	119.42	109.18
6	A	978	GOL	O1-C1-C2	2.40	121.20	110.38
6	A	970	GOL	O3-C3-C2	-2.35	99.81	110.38
6	A	975	GOL	O2-C2-C1	-2.32	99.59	109.18
6	A	970	GOL	O1-C1-C2	-2.04	101.20	110.38
6	A	975	GOL	C3-C2-C1	-2.02	104.38	111.80

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	970	GOL	O1-C1-C2-C3
6	A	972	GOL	O1-C1-C2-C3
6	A	973	GOL	O1-C1-C2-C3
6	A	973	GOL	C1-C2-C3-O3
6	A	977	GOL	O1-C1-C2-C3
6	A	978	GOL	C1-C2-C3-O3
6	A	978	GOL	O2-C2-C3-O3
6	A	979	GOL	O1-C1-C2-C3
6	A	981	GOL	O1-C1-C2-C3
6	A	982	GOL	C1-C2-C3-O3
6	A	972	GOL	O1-C1-C2-O2
6	A	973	GOL	O1-C1-C2-O2
6	A	973	GOL	O2-C2-C3-O3
6	A	975	GOL	O1-C1-C2-C3
6	A	976	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	A	981	GOL	C1-C2-C3-O3
6	A	970	GOL	O1-C1-C2-O2
6	A	979	GOL	O1-C1-C2-O2
6	A	981	GOL	O2-C2-C3-O3
6	A	982	GOL	O2-C2-C3-O3
6	A	976	GOL	O2-C2-C3-O3
6	A	977	GOL	O2-C2-C3-O3
6	A	972	GOL	O2-C2-C3-O3
6	A	983	GOL	O2-C2-C3-O3
6	A	983	GOL	O1-C1-C2-C3
6	A	978	GOL	O1-C1-C2-O2
6	A	979	GOL	O2-C2-C3-O3
5	A	950	MLI	C3-C1-C2-O7

There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	972	GOL	3	0
6	A	982	GOL	3	0
6	A	978	GOL	3	0
6	A	973	GOL	1	0
6	A	976	GOL	1	0
6	A	977	GOL	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 [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	866/891 (97%)	-0.94	1 (0%) 92 93	5, 12, 24, 46	62 (7%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	504	HIS	3.2

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(Å ²)	Q<0.9
6	GOL	A	983	6/6	0.67	0.24	27,33,35,35	6
6	GOL	A	982	6/6	0.71	0.25	31,34,35,35	6
6	GOL	A	981	6/6	0.85	0.16	24,27,32,34	6
6	GOL	A	977	6/6	0.89	0.16	27,29,30,35	6
6	GOL	A	978	6/6	0.90	0.12	11,21,25,33	6
6	GOL	A	976	6/6	0.92	0.16	12,23,30,31	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GOL	A	979	6/6	0.93	0.12	21,26,27,27	6
6	GOL	A	973	6/6	0.94	0.12	17,36,49,58	0
6	GOL	A	972	6/6	0.94	0.09	21,25,30,30	0
6	GOL	A	970	6/6	0.95	0.09	17,25,26,28	0
5	MLI	A	950	7/7	0.95	0.09	20,26,31,32	0
6	GOL	A	975	6/6	0.96	0.14	9,13,15,18	6
6	GOL	A	974	6/6	0.96	0.11	16,17,22,26	6
6	GOL	A	971	6/6	0.97	0.08	19,27,31,37	0
3	NA	A	892	1/1	0.99	0.19	21,21,21,21	1
4	SER	A	900	7/7	0.99	0.03	7,7,9,10	0
3	NA	A	890	1/1	1.00	0.07	15,15,15,15	0
3	NA	A	891	1/1	1.00	0.15	28,28,28,28	0
2	ZN	A	880	1/1	1.00	0.01	6,6,6,6	0

6.5 Other polymers [i](#)

There are no such residues in this entry.