



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:33 AM UTC

PDB ID : 4XND / pdb_00004xnd
Title : Crystal Structure of E. coli Aminopeptidase N in complex with L-Beta Homotryptophan
Authors : Addlagatta, A.; Gumpena, R.
Deposited on : 2015-01-15
Resolution : 1.93 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

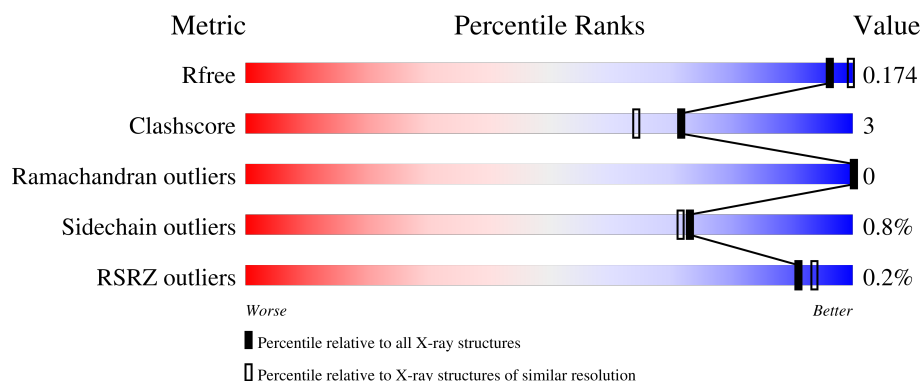
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	866	

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
6	MLI	A	933	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MLI	A	934	-	X	-	-
6	MLI	A	938	-	X	-	-
6	MLI	A	940	-	X	-	-
6	MLI	A	941	-	X	-	-
6	MLI	A	942	-	X	-	-
6	MLI	A	943	-	X	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8268 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.

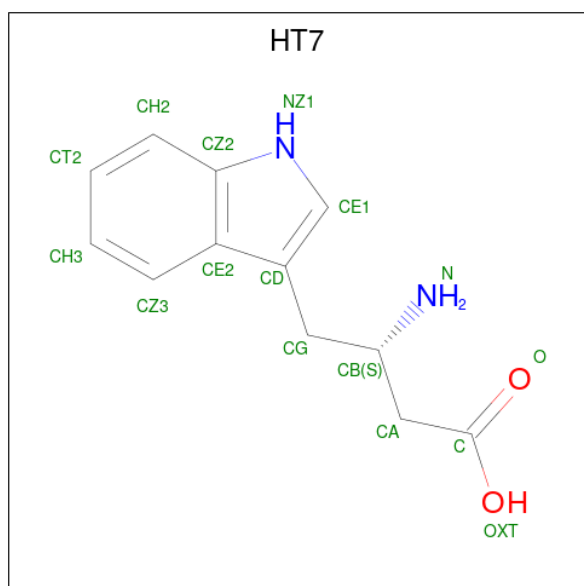
- Molecule 1 is a protein called Aminopeptidase N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	866	Total	C	N	O	S	0	30	0
			7122	4514	1237	1342	29			

- 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 (3S)-3-AMINO-4-(1H-INDOL-3-YL)BUTANOIC ACID (CCD ID: HT7) (formula: C₁₂H₁₄N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			16	12	2	2		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	Na	0	0
			8	8		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



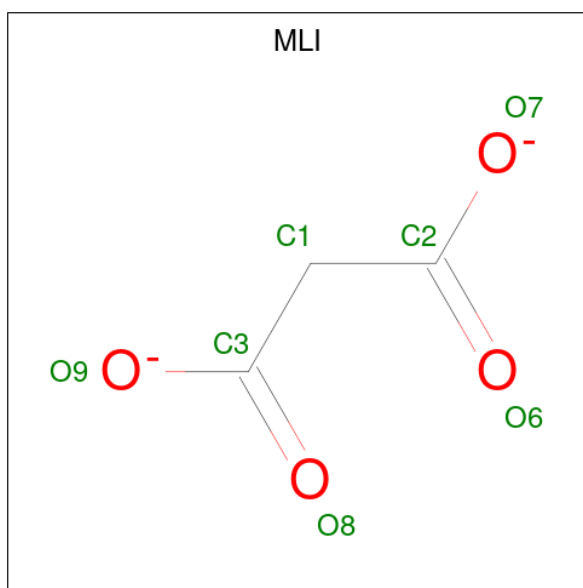
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	1
			12	6	6		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	1
			12	6	6		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 3 4	0	0
6	A	1	Total C O 7 3 4	0	0
6	A	1	Total C O 7 3 4	0	0
6	A	1	Total C O 7 3 4	0	0
6	A	1	Total C O 14 6 8	0	1
6	A	1	Total C O 7 3 4	0	0
6	A	1	Total C O 14 6 8	0	1
6	A	1	Total C O 7 3 4	0	0
6	A	1	Total C O 7 3 4	0	0
6	A	1	Total C O 7 3 4	0	0
6	A	1	Total C O 7 3 4	0	0
6	A	1	Total C O 7 3 4	0	0
6	A	1	Total C O 7 3 4	0	0
6	A	1	Total C O 7 3 4	0	0
6	A	1	Total C O 7 3 4	0	0

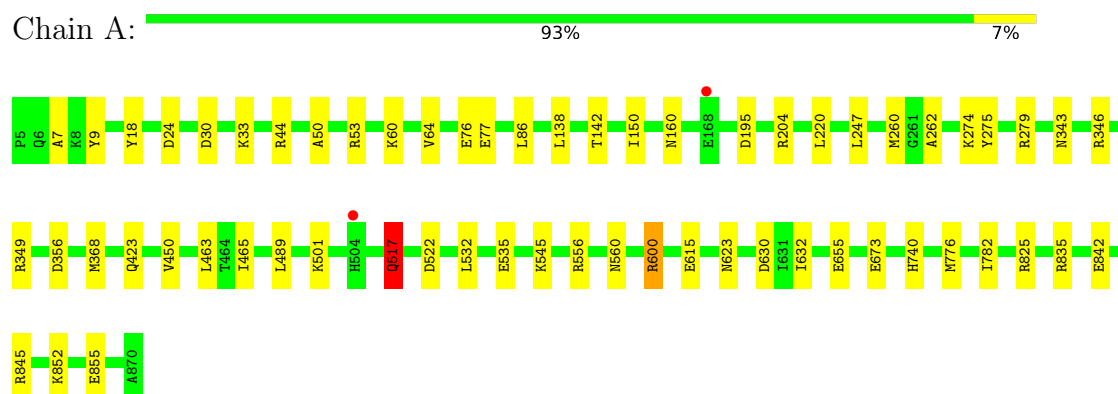
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	865	Total O 865 865	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 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	121.12Å 121.12Å 170.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.93 20.00 – 1.93	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-1.93) 99.0 (20.00-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 1.93Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.133 , 0.166 0.147 , 0.174	Depositor DCC
R_{free} test set	5384 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 67.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8268	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, MLI, HT7, NA

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	1.34	10/7364 (0.1%)	1.07	5/9988 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	349	ARG	CD-NE	-10.30	1.31	1.46
1	A	160	ASN	CG-ND2	-7.50	1.17	1.33
1	A	76	GLU	C-O	-6.37	1.16	1.24
1	A	623	ASN	CA-C	-6.23	1.44	1.52
1	A	489	LEU	CA-CB	-5.79	1.44	1.53
1	A	349	ARG	CZ-NH2	-5.57	1.26	1.33
1	A	517	GLN	CD-OE1	5.55	1.34	1.23
1	A	600	ARG	C-O	-5.32	1.18	1.24
1	A	532	LEU	CA-C	5.10	1.58	1.52
1	A	556	ARG	C-O	-5.02	1.17	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	ARG	NE-CZ-NH2	-8.51	111.55	119.20
1	A	64	VAL	CB-CA-C	-5.71	102.71	110.42
1	A	740	HIS	N-CA-C	5.39	118.65	111.75
1	A	50	ALA	CA-C-N	-5.14	115.43	120.52
1	A	50	ALA	C-N-CA	-5.14	115.43	120.52

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	7122	0	7037	42	0
2	A	1	0	0	0	0
3	A	16	0	13	2	0
4	A	8	0	0	0	0
5	A	144	0	191	7	0
6	A	112	0	32	5	0
7	A	865	0	0	19	2
All	All	8268	0	7273	49	2

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 (49) 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)
6:A:946:MLI:O6	7:A:1001:HOH:O	1.92	0.88
5:A:928[B]:GOL:O3	5:A:928[B]:GOL:O1	1.92	0.84
1:A:825:ARG:NH2	5:A:920:GOL:O3	2.31	0.64
6:A:943:MLI:O8	7:A:1002:HOH:O	2.14	0.64
5:A:923:GOL:O3	5:A:923:GOL:O1	2.18	0.62
1:A:517:GLN:OE1	7:A:1003:HOH:O	2.16	0.61
1:A:60:LYS:NZ	7:A:1012:HOH:O	2.34	0.60
1:A:204[B]:ARG:NH1	7:A:1005:HOH:O	2.23	0.58
1:A:346[B]:ARG:NH2	1:A:615:GLU:OE1	2.29	0.58
5:A:925:GOL:H32	7:A:1059:HOH:O	2.04	0.57
1:A:9:TYR:CE1	1:A:368[B]:MET:HG3	2.39	0.56
1:A:343:ASN:OD1	1:A:346[B]:ARG:NH1	2.39	0.56
1:A:835[A]:ARG:NH1	6:A:933:MLI:O9	2.39	0.55
1:A:845[B]:ARG:HD2	7:A:1006:HOH:O	2.06	0.55
1:A:835[B]:ARG:HD3	6:A:933:MLI:O9	2.07	0.54
1:A:630:ASP:O	1:A:835[B]:ARG:NH2	2.41	0.54
1:A:463[B]:LEU:HD23	1:A:465:ILE:HD11	1.90	0.54
1:A:142[B]:THR:HG23	7:A:1495:HOH:O	2.10	0.52
1:A:195:ASP:HB3	1:A:220:LEU:HG	1.93	0.51
1:A:24:ASP:HA	1:A:142[B]:THR:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ASP:OD1	1:A:142[B]:THR:HG22	2.12	0.50
1:A:274:LYS:HE3	1:A:275:TYR:CE2	2.47	0.49
1:A:501:LYS:HD2	1:A:522[A]:ASP:OD2	2.13	0.49
1:A:825:ARG:NH1	7:A:1015:HOH:O	2.35	0.48
1:A:44[A]:ARG:NH1	1:A:86:LEU:O	2.32	0.46
5:A:919:GOL:H31	7:A:1433:HOH:O	2.15	0.46
1:A:274:LYS:HD3	7:A:1118:HOH:O	2.15	0.46
1:A:262:ALA:O	3:A:902:HT7:HC2	2.17	0.45
1:A:673[A]:GLU:HG3	7:A:1387:HOH:O	2.15	0.45
1:A:138:LEU:HD12	1:A:138:LEU:N	2.33	0.44
1:A:247:LEU:HA	5:A:930:GOL:H31	1.99	0.44
1:A:855:GLU:HA	7:A:1054:HOH:O	2.18	0.44
1:A:545:LYS:NZ	7:A:1038:HOH:O	2.50	0.44
1:A:18:TYR:CZ	1:A:44[B]:ARG:HD3	2.53	0.43
5:A:919:GOL:C3	7:A:1433:HOH:O	2.66	0.43
1:A:18:TYR:OH	1:A:44[B]:ARG:HD3	2.19	0.43
1:A:423:GLN:NE2	7:A:1018:HOH:O	2.39	0.42
1:A:7:ALA:HB1	1:A:368[B]:MET:SD	2.60	0.42
1:A:450:VAL:CG1	1:A:463[B]:LEU:HD11	2.50	0.42
1:A:560:ASN:OD1	7:A:1004:HOH:O	2.22	0.41
1:A:845[A]:ARG:NH2	7:A:1011:HOH:O	2.29	0.41
1:A:150:ILE:HG12	7:A:1228:HOH:O	2.20	0.41
1:A:632:ILE:CD1	6:A:933:MLI:H11	2.50	0.41
1:A:53[A]:ARG:NH1	1:A:77:GLU:OE2	2.52	0.41
1:A:260:MET:HG3	3:A:902:HT7:CZ2	2.51	0.41
1:A:776:MET:O	1:A:782:ILE:HD11	2.21	0.40
1:A:30:ASP:HB3	1:A:33:LYS:O	2.21	0.40
1:A:600:ARG:HD3	1:A:655:GLU:OE2	2.21	0.40
1:A:24:ASP:OD1	1:A:142[B]:THR:CG2	2.69	0.40

All (2) 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)
7:A:1231:HOH:O	7:A:1231:HOH:O[6_554]	1.90	0.30
7:A:1701:HOH:O	7:A:1805:HOH:O[2_545]	2.18	0.02

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	894/866 (103%)	881 (98%)	13 (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	771/741 (104%)	763 (99%)	8 (1%)	68	64

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	279	ARG
1	A	356	ASP
1	A	517	GLN
1	A	535[A]	GLU
1	A	535[B]	GLU
1	A	842[A]	GLU
1	A	842[B]	GLU
1	A	852	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	A	479	GLN
1	A	504	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](#)

Of 50 ligands modelled in this entry, 9 are monoatomic - leaving 41 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	MLI	A	944	-	6,6,6	1.42	1 (16%)	7,7,7	0.75	0
6	MLI	A	946	4	6,6,6	1.68	1 (16%)	7,7,7	1.70	2 (28%)
5	GOL	A	917	-	5,5,5	0.27	0	5,5,5	0.48	0
6	MLI	A	940	-	6,6,6	1.53	1 (16%)	7,7,7	2.01	3 (42%)
6	MLI	A	941	-	6,6,6	2.32	2 (33%)	7,7,7	3.31	4 (57%)
5	GOL	A	916	-	5,5,5	0.24	0	5,5,5	0.97	0
6	MLI	A	943	-	6,6,6	1.66	2 (33%)	7,7,7	2.13	4 (57%)
6	MLI	A	934	-	6,6,6	2.90	3 (50%)	7,7,7	1.62	2 (28%)
5	GOL	A	926	-	5,5,5	1.48	1 (20%)	5,5,5	1.16	0
5	GOL	A	925	-	5,5,5	0.50	0	5,5,5	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MLI	A	935	-	6,6,6	1.41	1 (16%)	7,7,7	1.19	1 (14%)
5	GOL	A	928[A]	-	5,5,5	0.60	0	5,5,5	0.60	0
5	GOL	A	930	-	5,5,5	1.32	1 (20%)	5,5,5	2.34	3 (60%)
5	GOL	A	914	-	5,5,5	1.14	0	5,5,5	1.65	2 (40%)
3	HT7	A	902	2	17,17,17	1.71	5 (29%)	18,23,23	1.61	3 (16%)
5	GOL	A	928[B]	-	5,5,5	0.67	0	5,5,5	0.76	0
5	GOL	A	918	-	5,5,5	0.62	0	5,5,5	0.71	0
6	MLI	A	937[A]	-	6,6,6	1.43	1 (16%)	7,7,7	0.90	0
6	MLI	A	945	-	6,6,6	1.91	2 (33%)	7,7,7	1.53	2 (28%)
6	MLI	A	937[B]	-	6,6,6	1.05	1 (16%)	7,7,7	1.91	3 (42%)
5	GOL	A	922	-	5,5,5	0.36	0	5,5,5	0.78	0
5	GOL	A	924	-	5,5,5	0.49	0	5,5,5	1.45	1 (20%)
5	GOL	A	923	-	5,5,5	0.35	0	5,5,5	0.58	0
5	GOL	A	915	-	5,5,5	0.96	0	5,5,5	0.91	0
6	MLI	A	936	4	6,6,6	1.92	1 (16%)	7,7,7	1.97	2 (28%)
5	GOL	A	921	-	5,5,5	0.68	0	5,5,5	1.23	0
6	MLI	A	942	-	6,6,6	1.03	0	7,7,7	2.06	3 (42%)
5	GOL	A	911[A]	-	5,5,5	1.24	0	5,5,5	2.10	2 (40%)
5	GOL	A	920	-	5,5,5	0.76	0	5,5,5	1.62	2 (40%)
5	GOL	A	929	-	5,5,5	1.11	1 (20%)	5,5,5	2.10	2 (40%)
5	GOL	A	919	-	5,5,5	0.33	0	5,5,5	0.46	0
5	GOL	A	931	-	5,5,5	0.56	0	5,5,5	0.70	0
5	GOL	A	932	4	5,5,5	0.37	0	5,5,5	1.37	1 (20%)
6	MLI	A	939[A]	-	6,6,6	1.17	0	7,7,7	0.85	0
5	GOL	A	913	-	5,5,5	1.11	1 (20%)	5,5,5	1.47	1 (20%)
5	GOL	A	912	-	5,5,5	0.60	0	5,5,5	1.52	1 (20%)
5	GOL	A	927	-	5,5,5	0.64	0	5,5,5	1.24	0
5	GOL	A	911[B]	-	5,5,5	0.52	0	5,5,5	0.42	0
6	MLI	A	938	-	6,6,6	1.16	0	7,7,7	3.15	5 (71%)
6	MLI	A	939[B]	-	6,6,6	1.28	1 (16%)	7,7,7	1.99	3 (42%)
6	MLI	A	933	-	6,6,6	1.22	1 (16%)	7,7,7	1.11	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	MLI	A	944	-	-	0/4/4/4	-
6	MLI	A	946	4	-	0/4/4/4	-
5	GOL	A	917	-	-	3/4/4/4	-
6	MLI	A	940	-	-	4/4/4/4	-
6	MLI	A	941	-	-	2/4/4/4	-
5	GOL	A	916	-	-	4/4/4/4	-
6	MLI	A	943	-	-	4/4/4/4	-
6	MLI	A	934	-	-	2/4/4/4	-
5	GOL	A	926	-	-	2/4/4/4	-
5	GOL	A	925	-	-	4/4/4/4	-
6	MLI	A	935	-	-	2/4/4/4	-
5	GOL	A	928[A]	-	-	2/4/4/4	-
5	GOL	A	930	-	-	1/4/4/4	-
5	GOL	A	914	-	-	2/4/4/4	-
3	HT7	A	902	2	-	6/8/8/8	0/2/2/2
5	GOL	A	928[B]	-	-	4/4/4/4	-
5	GOL	A	918	-	-	3/4/4/4	-
6	MLI	A	937[A]	-	-	2/4/4/4	-
6	MLI	A	945	-	-	0/4/4/4	-
6	MLI	A	937[B]	-	-	2/4/4/4	-
5	GOL	A	922	-	-	1/4/4/4	-
5	GOL	A	924	-	-	2/4/4/4	-
5	GOL	A	923	-	-	2/4/4/4	-
5	GOL	A	915	-	-	0/4/4/4	-
6	MLI	A	936	4	-	0/4/4/4	-
5	GOL	A	921	-	-	4/4/4/4	-
6	MLI	A	942	-	-	4/4/4/4	-
5	GOL	A	911[A]	-	-	2/4/4/4	-
5	GOL	A	920	-	-	3/4/4/4	-
5	GOL	A	929	-	-	2/4/4/4	-
5	GOL	A	919	-	-	2/4/4/4	-
5	GOL	A	931	-	-	0/4/4/4	-
5	GOL	A	932	4	-	4/4/4/4	-
6	MLI	A	939[A]	-	-	4/4/4/4	-
5	GOL	A	913	-	-	1/4/4/4	-
5	GOL	A	912	-	-	2/4/4/4	-
5	GOL	A	927	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	911[B]	-	-	0/4/4/4	-
6	MLI	A	938	-	-	3/4/4/4	-
6	MLI	A	939[B]	-	-	0/4/4/4	-
6	MLI	A	933	-	-	1/4/4/4	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	934	MLI	C1-C2	-5.91	1.41	1.51
6	A	941	MLI	O8-C3	3.78	1.34	1.22
6	A	941	MLI	O9-C3	-3.27	1.20	1.30
6	A	945	MLI	O6-C2	3.24	1.32	1.22
3	A	902	HT7	O-C	3.22	1.32	1.22
6	A	936	MLI	C1-C2	3.22	1.56	1.51
6	A	934	MLI	O9-C3	-2.90	1.21	1.30
6	A	945	MLI	O9-C3	-2.65	1.22	1.30
3	A	902	HT7	CE1-CD	2.61	1.40	1.36
3	A	902	HT7	CH3-CZ3	2.52	1.43	1.38
3	A	902	HT7	OXT-C	-2.48	1.22	1.30
5	A	926	GOL	O2-C2	-2.45	1.36	1.43
6	A	946	MLI	O7-C2	-2.42	1.22	1.30
6	A	933	MLI	C1-C2	-2.41	1.47	1.51
6	A	937[A]	MLI	O6-C2	2.41	1.30	1.22
6	A	943	MLI	O6-C2	2.33	1.29	1.22
5	A	929	GOL	O2-C2	2.25	1.49	1.43
6	A	940	MLI	O6-C2	2.25	1.29	1.22
6	A	943	MLI	O9-C3	-2.24	1.23	1.30
6	A	934	MLI	O7-C2	-2.20	1.23	1.30
5	A	930	GOL	C1-C2	2.19	1.60	1.51
5	A	913	GOL	O2-C2	2.19	1.49	1.43
6	A	937[B]	MLI	O9-C3	-2.18	1.23	1.30
6	A	944	MLI	O6-C2	2.14	1.29	1.22
6	A	935	MLI	O7-C2	-2.11	1.23	1.30
3	A	902	HT7	CH2-CZ2	2.05	1.43	1.39
6	A	939[B]	MLI	C1-C2	-2.01	1.47	1.51

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	941	MLI	O9-C3-C1	-5.44	97.64	114.51
3	A	902	HT7	OXT-C-O	-4.82	110.94	123.33
6	A	938	MLI	O8-C3-C1	-4.70	108.72	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	941	MLI	O8-C3-C1	4.58	135.15	122.11
6	A	938	MLI	C3-C1-C2	-4.25	97.93	112.95
6	A	941	MLI	O6-C2-C1	-3.73	111.48	122.11
6	A	936	MLI	O7-C2-C1	3.59	125.63	114.51
5	A	930	GOL	O2-C2-C3	-3.47	94.81	109.18
6	A	943	MLI	O9-C3-C1	3.43	125.14	114.51
6	A	940	MLI	O8-C3-C1	-3.38	112.49	122.11
3	A	902	HT7	OXT-C-CA	3.22	124.01	114.00
6	A	938	MLI	O6-C2-C1	-3.18	113.05	122.11
5	A	929	GOL	O2-C2-C1	3.12	122.10	109.18
6	A	937[B]	MLI	O6-C2-C1	-3.11	113.27	122.11
5	A	911[A]	GOL	O1-C1-C2	3.04	124.07	110.38
6	A	940	MLI	O9-C3-C1	2.91	123.52	114.51
6	A	942	MLI	O8-C3-C1	-2.89	113.87	122.11
6	A	938	MLI	O7-C2-C1	2.87	123.41	114.51
6	A	942	MLI	O9-C3-C1	2.79	123.17	114.51
6	A	942	MLI	O6-C2-C1	-2.79	114.18	122.11
6	A	938	MLI	O9-C3-C1	2.78	123.14	114.51
6	A	939[B]	MLI	O6-C2-C1	-2.78	114.19	122.11
5	A	920	GOL	O1-C1-C2	-2.72	98.11	110.38
6	A	936	MLI	O7-C2-O6	-2.71	116.37	123.33
5	A	930	GOL	O2-C2-C1	-2.68	98.08	109.18
6	A	946	MLI	O7-C2-O6	-2.66	116.48	123.33
6	A	939[B]	MLI	O8-C3-C1	-2.64	114.59	122.11
5	A	911[A]	GOL	O2-C2-C3	-2.62	98.34	109.18
5	A	912	GOL	O3-C3-C2	2.61	122.14	110.38
5	A	929	GOL	C3-C2-C1	-2.59	102.28	111.80
6	A	937[B]	MLI	O7-C2-C1	2.50	122.26	114.51
5	A	930	GOL	C3-C2-C1	2.46	120.81	111.80
6	A	934	MLI	C3-C1-C2	-2.40	104.50	112.95
5	A	913	GOL	C3-C2-C1	-2.38	103.07	111.80
6	A	939[B]	MLI	C3-C1-C2	-2.32	104.76	112.95
6	A	946	MLI	O9-C3-C1	2.31	121.66	114.51
5	A	932	GOL	C3-C2-C1	2.28	120.17	111.80
6	A	943	MLI	C3-C1-C2	2.26	120.93	112.95
6	A	941	MLI	O7-C2-O6	2.24	129.10	123.33
6	A	943	MLI	O9-C3-O8	-2.23	117.61	123.33
5	A	914	GOL	O2-C2-C1	-2.21	100.02	109.18
5	A	914	GOL	O2-C2-C3	2.20	118.29	109.18
6	A	935	MLI	C3-C1-C2	-2.20	105.19	112.95
6	A	940	MLI	O6-C2-C1	-2.19	115.88	122.11
6	A	934	MLI	O7-C2-O6	2.17	128.91	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	943	MLI	O6-C2-C1	2.17	128.28	122.11
5	A	924	GOL	C3-C2-C1	-2.17	103.85	111.80
6	A	937[B]	MLI	O9-C3-C1	2.14	121.15	114.51
6	A	945	MLI	O9-C3-O8	-2.14	117.83	123.33
3	A	902	HT7	CD-CE1-NZ1	-2.11	107.99	110.31
6	A	945	MLI	O7-C2-C1	-2.09	108.03	114.51
5	A	920	GOL	O2-C2-C3	2.07	117.75	109.18

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	HT7	C-CA-CB-N
3	A	902	HT7	C-CA-CB-CG
5	A	911[A]	GOL	C1-C2-C3-O3
5	A	914	GOL	C1-C2-C3-O3
5	A	916	GOL	O1-C1-C2-O2
5	A	916	GOL	O1-C1-C2-C3
5	A	917	GOL	O1-C1-C2-C3
5	A	918	GOL	C1-C2-C3-O3
5	A	920	GOL	O1-C1-C2-C3
5	A	921	GOL	O1-C1-C2-O2
5	A	921	GOL	O1-C1-C2-C3
5	A	921	GOL	C1-C2-C3-O3
5	A	921	GOL	O2-C2-C3-O3
5	A	923	GOL	O1-C1-C2-C3
5	A	924	GOL	C1-C2-C3-O3
5	A	925	GOL	O1-C1-C2-C3
5	A	927	GOL	O1-C1-C2-C3
5	A	927	GOL	C1-C2-C3-O3
5	A	928[A]	GOL	O1-C1-C2-C3
5	A	928[B]	GOL	C1-C2-C3-O3
5	A	932	GOL	O1-C1-C2-C3
5	A	911[A]	GOL	O2-C2-C3-O3
5	A	928[A]	GOL	O1-C1-C2-O2
5	A	912	GOL	C1-C2-C3-O3
5	A	916	GOL	C1-C2-C3-O3
5	A	919	GOL	O1-C1-C2-C3
5	A	925	GOL	C1-C2-C3-O3
5	A	928[B]	GOL	O1-C1-C2-C3
5	A	929	GOL	O1-C1-C2-C3
5	A	932	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	A	917	GOL	O1-C1-C2-O2
5	A	923	GOL	O1-C1-C2-O2
5	A	927	GOL	O2-C2-C3-O3
5	A	928[B]	GOL	O2-C2-C3-O3
5	A	929	GOL	O1-C1-C2-O2
5	A	932	GOL	O1-C1-C2-O2
3	A	902	HT7	OXT-C-CA-CB
6	A	935	MLI	C2-C1-C3-O8
5	A	912	GOL	O2-C2-C3-O3
5	A	914	GOL	O2-C2-C3-O3
5	A	918	GOL	O2-C2-C3-O3
5	A	920	GOL	O1-C1-C2-O2
5	A	924	GOL	O2-C2-C3-O3
5	A	925	GOL	O2-C2-C3-O3
5	A	928[B]	GOL	O1-C1-C2-O2
3	A	902	HT7	O-C-CA-CB
6	A	935	MLI	C2-C1-C3-O9
5	A	916	GOL	O2-C2-C3-O3
5	A	925	GOL	O1-C1-C2-O2
5	A	932	GOL	O2-C2-C3-O3
6	A	937[A]	MLI	C3-C1-C2-O7
6	A	938	MLI	C3-C1-C2-O7
6	A	939[A]	MLI	C2-C1-C3-O9
6	A	940	MLI	C2-C1-C3-O9
5	A	913	GOL	O2-C2-C3-O3
5	A	918	GOL	O1-C1-C2-O2
6	A	940	MLI	C3-C1-C2-O7
6	A	940	MLI	C2-C1-C3-O8
6	A	942	MLI	C2-C1-C3-O8
5	A	920	GOL	C1-C2-C3-O3
5	A	926	GOL	O1-C1-C2-C3
6	A	937[A]	MLI	C3-C1-C2-O6
6	A	938	MLI	C3-C1-C2-O6
6	A	939[A]	MLI	C2-C1-C3-O8
6	A	942	MLI	C2-C1-C3-O9
5	A	919	GOL	O1-C1-C2-O2
5	A	927	GOL	O1-C1-C2-O2
6	A	937[B]	MLI	C3-C1-C2-O6
6	A	943	MLI	C2-C1-C3-O8
6	A	934	MLI	C2-C1-C3-O8
6	A	939[A]	MLI	C3-C1-C2-O6
6	A	939[A]	MLI	C3-C1-C2-O7

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Mol	Chain	Res	Type	Atoms
6	A	941	MLI	C3-C1-C2-O7
6	A	943	MLI	C3-C1-C2-O7
5	A	917	GOL	C1-C2-C3-O3
5	A	926	GOL	O1-C1-C2-O2
5	A	930	GOL	O2-C2-C3-O3
3	A	902	HT7	CE2-CD-CG-CB
6	A	934	MLI	C2-C1-C3-O9
6	A	941	MLI	C3-C1-C2-O6
6	A	943	MLI	C2-C1-C3-O9
6	A	937[B]	MLI	C3-C1-C2-O7
6	A	942	MLI	C3-C1-C2-O6
6	A	942	MLI	C3-C1-C2-O7
6	A	943	MLI	C3-C1-C2-O6
3	A	902	HT7	CE1-CD-CG-CB
6	A	940	MLI	C3-C1-C2-O6
5	A	922	GOL	O1-C1-C2-O2
6	A	933	MLI	C3-C1-C2-O6
6	A	938	MLI	C2-C1-C3-O8

There are no ring outliers.

10 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	946	MLI	1	0
6	A	943	MLI	1	0
5	A	925	GOL	1	0
5	A	930	GOL	1	0
3	A	902	HT7	2	0
5	A	928[B]	GOL	1	0
5	A	923	GOL	1	0
5	A	920	GOL	1	0
5	A	919	GOL	2	0
6	A	933	MLI	3	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	866/866 (100%)	-0.56	2 (0%) 91 94	10, 20, 38, 71	30 (3%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	168	GLU	2.5
1	A	504	HIS	2.4

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	MLI	A	941	7/7	0.76	0.21	40,58,63,64	0
6	MLI	A	946	7/7	0.76	0.19	47,65,71,96	0
6	MLI	A	935	7/7	0.77	0.14	65,73,74,77	0
5	GOL	A	923	6/6	0.79	0.19	67,73,81,81	0
6	MLI	A	944	7/7	0.81	0.15	64,69,78,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	A	929	6/6	0.81	0.15	37,50,56,58	0
5	GOL	A	931	6/6	0.82	0.21	58,70,72,84	0
6	MLI	A	939[A]	7/7	0.82	0.19	64,68,73,87	7
6	MLI	A	939[B]	7/7	0.82	0.19	16,17,19,23	7
6	MLI	A	945	7/7	0.84	0.17	54,62,65,76	0
5	GOL	A	924	6/6	0.85	0.15	47,53,58,59	0
5	GOL	A	928[A]	6/6	0.85	0.14	27,45,49,56	6
6	MLI	A	940	7/7	0.85	0.14	36,50,66,77	0
5	GOL	A	928[B]	6/6	0.85	0.14	33,43,45,52	6
6	MLI	A	937[A]	7/7	0.85	0.17	41,50,55,63	7
6	MLI	A	937[B]	7/7	0.85	0.17	29,31,37,43	7
6	MLI	A	938	7/7	0.85	0.19	49,67,70,86	0
5	GOL	A	920	6/6	0.86	0.15	39,45,54,54	0
6	MLI	A	942	7/7	0.86	0.18	54,57,73,93	0
5	GOL	A	921	6/6	0.86	0.15	44,45,53,54	0
5	GOL	A	922	6/6	0.86	0.16	46,56,60,70	0
5	GOL	A	919	6/6	0.86	0.14	58,63,69,70	0
5	GOL	A	925	6/6	0.87	0.15	35,54,63,77	0
6	MLI	A	943	7/7	0.88	0.11	34,40,58,66	0
5	GOL	A	911[B]	6/6	0.88	0.15	7,8,8,8	6
5	GOL	A	930	6/6	0.88	0.16	27,34,45,49	0
5	GOL	A	911[A]	6/6	0.88	0.15	34,39,50,51	6
6	MLI	A	934	7/7	0.90	0.13	31,40,59,63	0
5	GOL	A	916	6/6	0.90	0.11	52,55,57,59	0
6	MLI	A	933	7/7	0.91	0.15	26,37,38,43	0
5	GOL	A	914	6/6	0.91	0.12	27,32,35,35	0
5	GOL	A	932	6/6	0.91	0.11	44,53,58,61	0
4	NA	A	905	1/1	0.92	0.13	53,53,53,53	0
5	GOL	A	913	6/6	0.92	0.10	35,38,49,60	0
5	GOL	A	917	6/6	0.93	0.10	27,49,52,56	0
6	MLI	A	936	7/7	0.93	0.17	25,34,50,54	0
5	GOL	A	918	6/6	0.94	0.11	34,39,44,45	0
5	GOL	A	927	6/6	0.94	0.12	35,37,47,49	0
5	GOL	A	912	6/6	0.96	0.08	21,37,41,43	0
4	NA	A	906	1/1	0.96	0.07	39,39,39,39	0
4	NA	A	909	1/1	0.96	0.07	43,43,43,43	0
4	NA	A	908	1/1	0.97	0.14	32,32,32,32	0
4	NA	A	904	1/1	0.97	0.06	30,30,30,30	0
5	GOL	A	915	6/6	0.97	0.05	19,23,24,27	0
4	NA	A	910	1/1	0.97	0.16	33,33,33,33	0
5	GOL	A	926	6/6	0.98	0.07	22,25,28,30	0
3	HT7	A	902	16/16	0.98	0.05	12,17,19,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NA	A	907	1/1	0.99	0.10	22,22,22,22	0
4	NA	A	903	1/1	0.99	0.04	21,21,21,21	0
2	ZN	A	901	1/1	1.00	0.02	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.