



wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 02:57 AM GMT

PDB ID : 1A4M
Title : ADA STRUCTURE COMPLEXED WITH PURINE RIBOSIDE AT PH 7.0
Authors : Wang, Z.; Quioco, F.A.
Deposited on : 1998-01-31
Resolution : 1.95 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

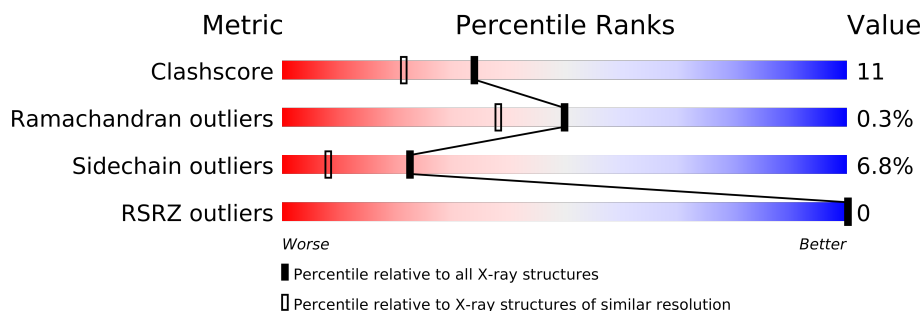
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.95 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))
Clashscore	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)
RSRZ outliers	66119	1321 (1.96-1.96)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	349	
1	B	349	
1	C	349	
1	D	349	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12313 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

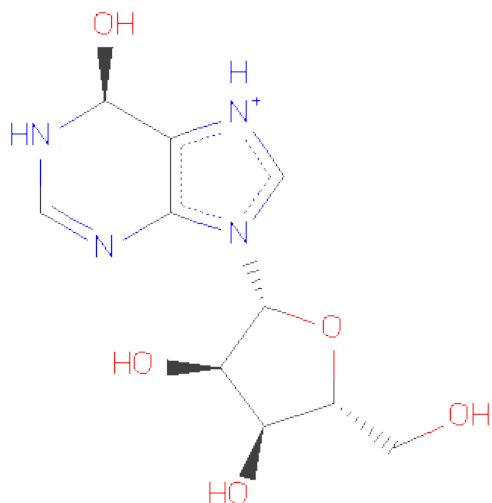
- Molecule 1 is a protein called ADENOSINE DEAMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2792	1778	470	530	14			
1	B	349	Total	C	N	O	S	0	0	0
			2792	1778	470	530	14			
1	C	349	Total	C	N	O	S	0	0	0
			2792	1778	470	530	14			
1	D	349	Total	C	N	O	S	0	0	0
			2792	1778	470	530	14			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is 6-HYDROXY-1,6-DIHYDROPURINE NUCLEOSIDE (three-letter code: PRH) (formula: C₁₀H₁₅N₄O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	10	4	5		
3	B	1	Total	C	N	O	0	0
			19	10	4	5		
3	C	1	Total	C	N	O	0	0
			19	10	4	5		
3	D	1	Total	C	N	O	0	0
			19	10	4	5		

- Molecule 4 is water.

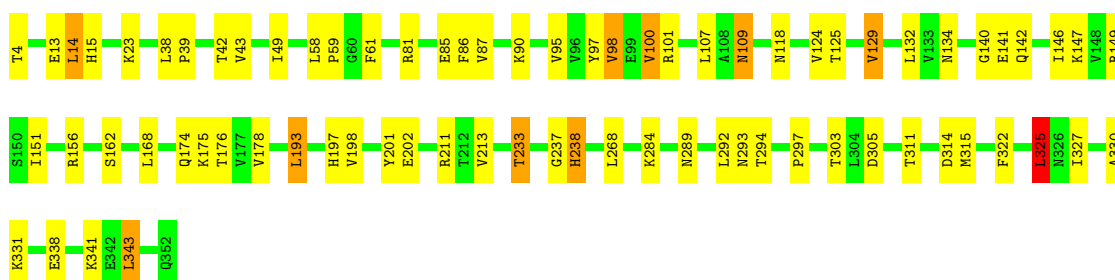
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	287	Total	O	0	0
			287	287		
4	B	269	Total	O	0	0
			269	269		
4	C	242	Total	O	0	0
			242	242		
4	D	267	Total	O	0	0
			267	267		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

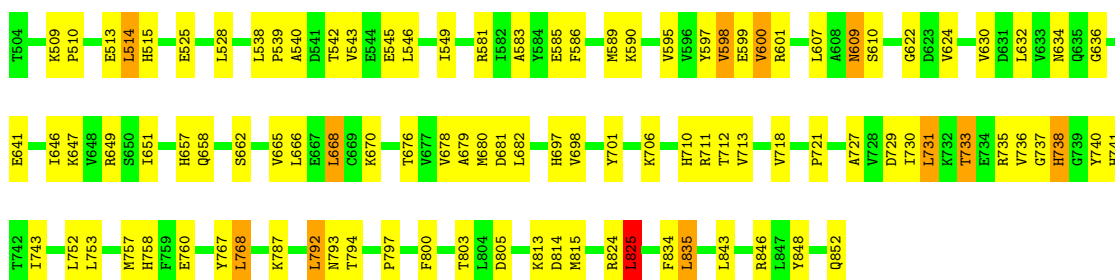
• Molecule 1: ADENOSINE DEAMINASE

Chain A:



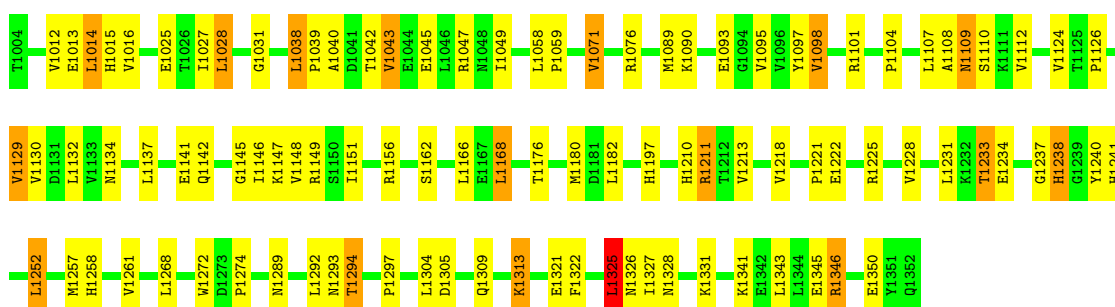
• Molecule 1: ADENOSINE DEAMINASE

Chain B:



• Molecule 1: ADENOSINE DEAMINASE

Chain C:



• Molecule 1: ADENOSINE DEAMINASE

Chain D: 

T1504	L1632	H1778	T1803	P1797	H1517	Y1529	R1649	D1805	D1814	F1822	L1825	N1826	I1827	K1831	L1835	E1838	E1839	L1843	R1846	L1847	Y1848	Q1852	E1593	G1594	V1595	V1598	E1599	V1600	R1601	L1607	A1608	N1609	V1612	H1617	N1618	Q1619	V1624	T1625	P1626	V1629	V1630	D1631
K1511	V1633	L1792	L1804	T1794	K1512	K1532	H1657	M1815	M1815	L1822	L1825	N1826	I1827	K1831	L1835	E1838	E1839	L1843	R1846	L1847	Y1848	Q1852	G1594	V1595	V1598	E1599	V1600	R1601	L1607	A1608	N1609	V1612	H1617	N1618	Q1619	V1624	T1625	P1626	V1629	V1630	D1631	
E1513	Q1635	L1793	D1805	T1794	E1514	K1532	H1657	M1815	M1815	L1822	L1825	N1826	I1827	K1831	L1835	E1838	E1839	L1843	R1846	L1847	Y1848	Q1852	G1594	V1595	V1598	E1599	V1600	R1601	L1607	A1608	N1609	V1612	H1617	N1618	Q1619	V1624	T1625	P1626	V1629	V1630	D1631	
L1514	E1641	T1794	D1805	T1794	L1514	K1532	H1657	M1815	M1815	L1822	L1825	N1826	I1827	K1831	L1835	E1838	E1839	L1843	R1846	L1847	Y1848	Q1852	G1594	V1595	V1598	E1599	V1600	R1601	L1607	A1608	N1609	V1612	H1617	N1618	Q1619	V1624	T1625	P1626	V1629	V1630	D1631	
H1517	I1646	P1797	L1803	P1797	H1517	Y1529	R1649	D1805	D1814	F1822	L1825	N1826	I1827	K1831	L1835	E1838	E1839	L1843	R1846	L1847	Y1848	Q1852	E1593	G1594	V1595	V1598	E1599	V1600	R1601	L1607	A1608	N1609	V1612	H1617	N1618	Q1619	V1624	T1625	P1626	V1629	V1630	D1631

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.69Å 93.64Å 102.18Å 90.00° 102.84° 90.00°	Depositor
Resolution (Å)	10.00 – 1.95 39.56 – 1.95	Depositor EDS
% Data completeness (in resolution range)	70.2 (10.00-1.95) 65.7 (39.56-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 1.95Å)	Xtriage
Refinement program	X-PLOR 3.85	Depositor
R, R_{free}	0.193 , 0.281 0.199 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	16.3	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 77949 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12313	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 62.96 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.0400e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PRH

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	0.41	0/2856	0.69	1/3864 (0.0%)
1	B	0.42	0/2856	0.70	3/3864 (0.1%)
1	C	0.41	0/2856	0.69	1/3864 (0.0%)
1	D	0.42	0/2856	0.68	1/3864 (0.0%)
All	All	0.42	0/11424	0.69	6/15456 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1825	LEU	CA-CB-CG	8.66	135.22	115.30
1	A	325	LEU	CA-CB-CG	8.64	135.16	115.30
1	C	1325	LEU	CA-CB-CG	7.89	133.44	115.30
1	B	825	LEU	CA-CB-CG	7.54	132.63	115.30
1	B	835	LEU	CA-CB-CG	5.98	129.06	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2792	0	2757	50	0
1	B	2792	0	2757	69	0
1	C	2792	0	2757	66	0
1	D	2792	0	2757	62	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	19	0	14	2	0
3	B	19	0	14	0	0
3	C	19	0	14	0	0
3	D	19	0	14	1	0
4	A	287	0	0	10	0
4	B	269	0	0	2	0
4	C	242	0	0	10	0
4	D	267	0	0	3	0
All	All	12313	0	11084	244	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

The worst 5 of 244 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:528:LEU:HD13	1:B:546:LEU:HD22	1.55	0.89
1:C:1109:ASN:HD21	1:C:1124:VAL:H	1.22	0.87
1:A:294:THR:HG23	1:A:297:PRO:HD3	1.59	0.83
1:C:1294:THR:HG23	1:C:1297:PRO:HD3	1.62	0.80
1:B:792:LEU:HD22	1:B:825:LEU:HD11	1.66	0.77

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	347/349 (99%)	334 (96%)	12 (4%)	1 (0%)	50 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	347/349 (99%)	335 (96%)	11 (3%)	1 (0%)	50	38
1	C	347/349 (99%)	333 (96%)	13 (4%)	1 (0%)	50	38
1	D	347/349 (99%)	334 (96%)	12 (4%)	1 (0%)	50	38
All	All	1388/1396 (99%)	1336 (96%)	48 (4%)	4 (0%)	50	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1238	HIS
1	A	238	HIS
1	B	738	HIS
1	D	1738	HIS

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	304/304 (100%)	283 (93%)	21 (7%)	22	8
1	B	304/304 (100%)	286 (94%)	18 (6%)	28	12
1	C	304/304 (100%)	281 (92%)	23 (8%)	19	6
1	D	304/304 (100%)	283 (93%)	21 (7%)	22	8
All	All	1216/1216 (100%)	1133 (93%)	83 (7%)	22	8

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	843	LEU
1	C	1109	ASN
1	D	1752	LEU
1	B	846	ARG
1	C	1043	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	756	ASN
1	C	1119	GLN
1	D	1756	ASN
1	B	789	ASN
1	B	826	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	PRH	A	354	2	21,21,21	5.75	4 (19%)	29,31,31	2.68	9 (31%)
3	PRH	B	854	2	21,21,21	5.70	4 (19%)	29,31,31	2.67	9 (31%)
3	PRH	C	1354	2	21,21,21	5.61	4 (19%)	29,31,31	2.50	9 (31%)
3	PRH	D	1854	2	21,21,21	5.64	4 (19%)	29,31,31	2.65	10 (34%)

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	PRH	A	354	2	-	0/6/32/32	0/1/3/3
3	PRH	B	854	2	-	0/6/32/32	0/1/3/3
3	PRH	C	1354	2	-	0/6/32/32	0/1/3/3
3	PRH	D	1854	2	-	0/6/32/32	0/1/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	354	PRH	O6-C6	25.39	1.61	1.41
3	B	854	PRH	O6-C6	25.23	1.61	1.41
3	D	1854	PRH	O6-C6	24.95	1.60	1.41
3	C	1354	PRH	O6-C6	24.86	1.60	1.41
3	A	354	PRH	C5-C6	-3.92	1.44	1.52

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	854	PRH	C2'-C3'-C4'	-6.79	89.11	102.65
3	A	354	PRH	C2'-C3'-C4'	-6.76	89.18	102.65
3	D	1854	PRH	C2'-C3'-C4'	-6.68	89.35	102.65
3	C	1354	PRH	C3'-C2'-C1'	5.91	110.15	100.91
3	A	354	PRH	C3'-C2'-C1'	5.89	110.13	100.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	349/349 (100%)	-0.42	0 100 100	8, 16, 29, 44	0
1	B	349/349 (100%)	-0.41	0 100 100	7, 15, 29, 44	0
1	C	349/349 (100%)	-0.40	0 100 100	7, 16, 28, 44	0
1	D	349/349 (100%)	-0.36	0 100 100	8, 16, 29, 43	0
All	All	1396/1396 (100%)	-0.40	0 100 100	7, 16, 29, 44	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	PRH	B	854	19/19	0.07	-0.33	5,9,13,14	0
3	PRH	A	354	19/19	0.08	-0.37	5,10,15,19	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	PRH	D	1854	19/19	0.07	-0.55	3,8,11,12	0
3	PRH	C	1354	19/19	0.08	-0.55	2,10,14,17	0
2	ZN	B	900	1/1	0.08	-0.90	16,16,16,16	0
2	ZN	D	1900	1/1	0.07	-1.66	16,16,16,16	0
2	ZN	C	1400	1/1	0.07	-1.87	15,15,15,15	0
2	ZN	A	400	1/1	0.06	-1.98	13,13,13,13	0

6.5 Other polymers ⓘ

There are no such residues in this entry.