Full wwPDB Geometry-Only Validation Report

Aug 31, 2020 – 10:19 AM BST

PDB ID	:	1FUB
Title	:	FIRST PROTEIN STRUCTURE DETERMINED FROM X-RAY POWDER DIFFRACTION DATA
Authors	:	Von Dreele, R.B.; Stephens, P.W.; Blessing, R.H.; Smith, G.D.
Deposited on	:	2000-09-14
Resolution	:	Not provided

This is a Full wwPDB Geometry-Only 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

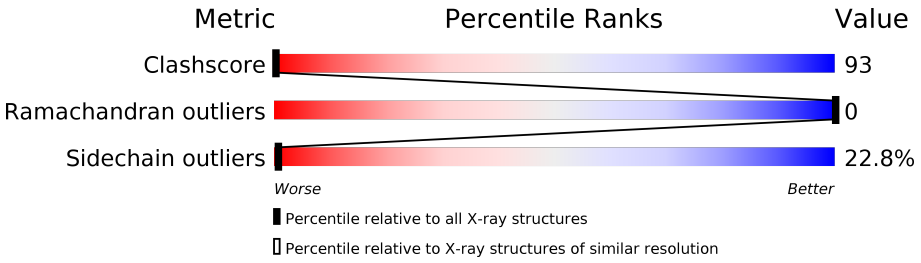
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
POWDER DIFFRACTION

The reported resolution of this entry is unknown.

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	141614	-
Ramachandran outliers	138981	-
Sidechain outliers	138945	-

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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	21	24% 57% 19%
1	C	21	19% 67% 14%
2	B	30	23% 67% 10%
2	D	30	30% 50% 20%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 815 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 INSULIN, A CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	C	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			

- Molecule 2 is a protein called INSULIN, B CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	30	Total	C	N	O	S	0	0	0
			242	158	40	42	2			
2	D	30	Total	C	N	O	S	0	0	0
			242	158	40	42	2			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Na 1 1	0	0

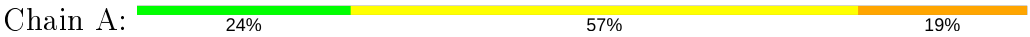
3 Residue-property plots (i)

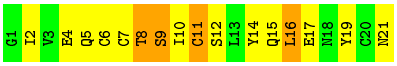
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

- Molecule 1: INSULIN, A CHAIN

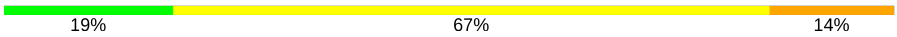
Chain A:

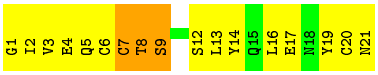




- Molecule 1: INSULIN, A CHAIN

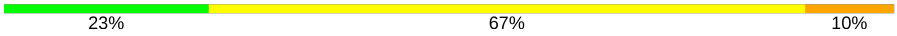
Chain C:





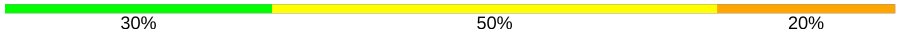
- Molecule 2: INSULIN, B CHAIN

Chain B:



- Molecule 2: INSULIN, B CHAIN

Chain D:



4 Model quality

4.1 Standard geometry

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

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	0.32	0/164	0.73	0/220
1	C	0.37	0/164	0.72	0/220
2	B	0.37	0/249	0.77	0/335
2	D	0.42	0/249	0.74	0/335
All	All	0.38	0/826	0.75	0/1110

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	22	ARG	Sidechain
2	D	22	ARG	Sidechain

4.2 Too-close contacts (i)

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	163	0	149	35	0
1	C	163	0	149	34	0
2	B	242	0	232	71	0
2	D	242	0	232	48	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	B	1	0	0	0	0
All	All	815	0	762	146	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 93.

All (146) 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:2:ILE:HG22	2:D:30:THR:O	1.41	1.18
2:B:16:TYR:HA	2:B:24:PHE:CE2	1.89	1.06
2:B:6:LEU:HD13	2:B:11:LEU:HD13	1.32	1.05
1:A:11:CYS:SG	1:A:16:LEU:HD11	2.05	0.97
2:B:6:LEU:CD1	2:B:11:LEU:HD13	1.95	0.97
2:B:6:LEU:HD13	2:B:11:LEU:CD1	1.94	0.97
2:D:8:GLY:O	2:D:12:VAL:HG22	1.67	0.95
1:C:1:GLY:HA3	1:C:4:GLU:HG3	1.48	0.92
1:C:1:GLY:CA	1:C:4:GLU:HG3	2.01	0.89
2:D:7:CYS:O	2:D:11:LEU:HG	1.70	0.89
2:B:6:LEU:HB3	2:B:11:LEU:HD22	1.51	0.89
2:B:26:TYR:CE2	2:B:28:PRO:HG3	2.07	0.89
1:A:14:TYR:HD1	1:A:17:GLU:HG3	1.37	0.88
1:C:1:GLY:O	1:C:5:GLN:HG2	1.74	0.88
2:D:16:TYR:HA	2:D:24:PHE:CE1	2.10	0.86
2:B:6:LEU:CG	2:B:11:LEU:HD13	2.06	0.85
2:B:28:PRO:HD3	2:D:23:GLY:HA3	1.58	0.85
1:A:2:ILE:HD12	1:A:19:TYR:CD1	2.13	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:GLU:HA	1:A:8:THR:HB	1.59	0.82
2:D:4:GLN:HA	2:D:7:CYS:HB2	1.61	0.82
2:B:6:LEU:CB	2:B:11:LEU:HD22	2.09	0.82
1:A:16:LEU:HA	1:A:19:TYR:HD2	1.45	0.81
2:B:16:TYR:HB2	2:B:24:PHE:CZ	2.15	0.81
1:A:16:LEU:HD13	1:A:16:LEU:N	1.93	0.80
1:A:15:GLN:O	1:A:19:TYR:CE2	2.36	0.79
1:C:3:VAL:O	1:C:7:CYS:HB2	1.83	0.78
1:A:4:GLU:HA	1:A:8:THR:CB	2.13	0.78
1:A:14:TYR:CD1	1:A:17:GLU:HG3	2.18	0.78
1:A:16:LEU:HA	1:A:19:TYR:CD2	2.19	0.77
1:A:7:CYS:HB2	2:B:6:LEU:O	1.85	0.77
2:B:6:LEU:HB3	2:B:11:LEU:CD2	2.14	0.77
1:C:6:CYS:HA	1:C:9:SER:O	1.86	0.76
2:B:25:PHE:HB3	2:D:25:PHE:CE2	2.22	0.75
1:A:2:ILE:HD12	1:A:19:TYR:CE1	2.22	0.75
2:B:6:LEU:HB3	2:B:11:LEU:CG	2.17	0.75
2:B:6:LEU:HB3	2:B:11:LEU:HB2	1.69	0.75
1:A:2:ILE:O	1:A:5:GLN:HB2	1.86	0.74
1:A:6:CYS:SG	1:A:16:LEU:HD11	2.27	0.74
2:B:28:PRO:HG2	2:D:23:GLY:N	2.02	0.73
1:A:4:GLU:CA	1:A:8:THR:HB	2.19	0.72
1:C:5:GLN:HG3	1:C:19:TYR:OH	1.89	0.72
1:C:1:GLY:H3	1:C:4:GLU:HG3	1.55	0.72
2:B:1:PHE:CE2	2:B:2:VAL:O	2.44	0.71
2:B:28:PRO:CD	2:D:23:GLY:HA3	2.21	0.71
2:B:6:LEU:HD22	2:B:11:LEU:HD13	1.71	0.70
1:C:1:GLY:N	1:C:4:GLU:HG3	2.06	0.70
1:A:11:CYS:SG	1:A:16:LEU:CD1	2.81	0.69
1:A:15:GLN:O	1:A:19:TYR:HE2	1.73	0.69
2:B:6:LEU:CD2	2:B:11:LEU:HD13	2.23	0.69
2:B:28:PRO:HD3	2:D:23:GLY:CA	2.23	0.68
2:B:6:LEU:HD22	2:B:11:LEU:CD1	2.24	0.68
2:B:28:PRO:CD	2:D:23:GLY:CA	2.72	0.67
1:A:2:ILE:CD1	1:A:19:TYR:CD1	2.78	0.66
2:D:16:TYR:HA	2:D:24:PHE:CZ	2.30	0.66
2:B:6:LEU:CB	2:B:11:LEU:HD13	2.24	0.66
2:B:6:LEU:HB3	2:B:11:LEU:CB	2.26	0.66
1:C:21:ASN:HD21	2:D:25:PHE:HD1	1.43	0.66
1:C:5:GLN:HA	1:C:5:GLN:OE1	1.95	0.65
2:B:6:LEU:HB3	2:B:11:LEU:HD13	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ILE:HA	2:B:4:GLN:O	1.96	0.65
2:D:1:PHE:HD1	2:D:1:PHE:H3	1.46	0.63
1:A:6:CYS:O	1:A:9:SER:O	2.17	0.63
1:A:21:ASN:OD1	2:B:25:PHE:HD2	1.80	0.63
2:B:28:PRO:HB2	2:D:21:GLU:HA	1.80	0.63
2:B:16:TYR:HA	2:B:24:PHE:CZ	2.33	0.62
2:D:16:TYR:HA	2:D:24:PHE:HE1	1.63	0.62
2:B:16:TYR:HB2	2:B:24:PHE:HZ	1.63	0.62
1:C:13:LEU:HD23	1:C:13:LEU:C	2.19	0.62
1:A:16:LEU:N	1:A:16:LEU:CD1	2.63	0.62
2:B:28:PRO:CG	2:D:23:GLY:CA	2.78	0.61
1:C:16:LEU:HD12	2:D:18:VAL:HG21	1.81	0.61
2:B:28:PRO:CB	2:D:21:GLU:HA	2.29	0.61
2:B:1:PHE:CD2	2:B:2:VAL:O	2.53	0.61
2:B:25:PHE:HB3	2:D:25:PHE:CD2	2.36	0.61
2:B:29:LYS:O	2:B:30:THR:OXT	2.19	0.60
2:B:28:PRO:HG2	2:D:21:GLU:C	2.22	0.60
2:B:27:THR:O	2:B:27:THR:OG1	2.18	0.60
2:B:13:GLU:OE1	2:D:12:VAL:HG23	2.02	0.59
1:C:1:GLY:HA3	1:C:4:GLU:CG	2.26	0.59
2:D:8:GLY:O	2:D:12:VAL:CG2	2.47	0.59
1:A:6:CYS:SG	1:A:16:LEU:CD1	2.90	0.58
1:C:2:ILE:CG2	2:D:30:THR:O	2.34	0.58
2:B:8:GLY:C	2:B:10:HIS:H	2.07	0.58
2:B:28:PRO:HG2	2:D:21:GLU:O	2.04	0.58
1:A:2:ILE:CD1	1:A:19:TYR:CE1	2.86	0.58
2:D:16:TYR:CD1	2:D:16:TYR:C	2.74	0.58
2:B:13:GLU:O	2:B:17:LEU:HB2	2.03	0.57
2:B:6:LEU:HB3	2:B:11:LEU:CD1	2.33	0.57
2:B:25:PHE:CB	2:D:25:PHE:CE2	2.88	0.57
2:B:13:GLU:OE2	2:D:9:SER:HB3	2.05	0.56
2:B:28:PRO:CG	2:D:23:GLY:HA2	2.35	0.56
2:B:13:GLU:OE2	2:D:9:SER:CB	2.53	0.56
1:C:1:GLY:CA	1:C:4:GLU:CG	2.79	0.56
1:C:1:GLY:O	1:C:4:GLU:HB2	2.06	0.56
2:B:28:PRO:HB2	2:D:21:GLU:O	2.07	0.54
2:B:13:GLU:O	2:B:17:LEU:CB	2.56	0.54
1:C:1:GLY:O	1:C:5:GLN:N	2.41	0.53
1:C:6:CYS:CA	1:C:9:SER:O	2.56	0.53
1:A:7:CYS:CB	2:B:6:LEU:O	2.57	0.53
1:C:1:GLY:N	1:C:4:GLU:HB2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:PRO:CG	2:D:21:GLU:O	2.59	0.51
2:D:19:CYS:HB2	2:D:24:PHE:CD1	2.45	0.51
1:C:2:ILE:HD12	1:C:19:TYR:CG	2.46	0.51
2:B:13:GLU:OE2	2:D:9:SER:HA	2.10	0.51
1:C:6:CYS:C	1:C:9:SER:O	2.50	0.50
1:C:17:GLU:HA	1:C:20:CYS:SG	2.51	0.50
1:A:15:GLN:O	1:A:19:TYR:CD2	2.64	0.50
1:C:20:CYS:O	1:C:21:ASN:C	2.50	0.50
1:A:8:THR:O	2:B:5:HIS:CE1	2.65	0.49
2:B:13:GLU:OE2	2:D:9:SER:CA	2.60	0.49
2:B:6:LEU:CB	2:B:11:LEU:HB2	2.42	0.49
2:B:16:TYR:CD2	2:B:17:LEU:N	2.81	0.49
1:A:16:LEU:CA	1:A:19:TYR:HD2	2.21	0.48
2:B:16:TYR:CB	2:B:24:PHE:CZ	2.90	0.48
2:D:29:LYS:O	2:D:30:THR:HG23	2.13	0.48
1:C:8:THR:HG23	2:D:2:VAL:HG21	1.96	0.48
1:C:5:GLN:CA	1:C:5:GLN:OE1	2.61	0.47
1:A:6:CYS:C	1:A:9:SER:O	2.53	0.47
1:A:21:ASN:OD1	2:B:25:PHE:CD2	2.65	0.47
1:C:21:ASN:ND2	2:D:24:PHE:HA	2.29	0.47
2:B:6:LEU:HB2	2:B:11:LEU:HD22	1.94	0.46
2:B:12:VAL:HG13	2:B:13:GLU:N	2.31	0.45
2:D:1:PHE:CD1	2:D:1:PHE:N	2.82	0.45
2:B:24:PHE:CZ	2:D:26:TYR:CD2	3.04	0.45
1:C:21:ASN:ND2	2:D:25:PHE:HD1	2.12	0.45
2:B:1:PHE:CG	2:B:2:VAL:N	2.85	0.45
2:B:28:PRO:HG3	2:D:23:GLY:HA2	1.99	0.45
2:B:16:TYR:CA	2:B:24:PHE:CZ	3.00	0.45
1:A:4:GLU:C	1:A:8:THR:HB	2.37	0.44
1:A:6:CYS:HB3	1:A:11:CYS:HB2	1.80	0.44
2:B:14:ALA:O	2:B:18:VAL:N	2.46	0.44
2:B:13:GLU:OE1	2:D:12:VAL:CG2	2.65	0.43
1:C:13:LEU:O	1:C:13:LEU:HD23	2.18	0.43
1:A:15:GLN:C	1:A:16:LEU:HD13	2.40	0.42
2:D:15:LEU:O	2:D:16:TYR:C	2.56	0.42
1:C:1:GLY:H3	1:C:4:GLU:CG	2.28	0.42
1:A:10:ILE:HG23	2:B:4:GLN:O	2.19	0.42
1:A:9:SER:HA	2:B:5:HIS:CE1	2.55	0.41
2:B:6:LEU:HD13	2:B:11:LEU:HD11	1.92	0.41
1:C:2:ILE:HG23	1:C:3:VAL:N	2.35	0.41
1:C:1:GLY:O	1:C:4:GLU:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:GLY:H2	1:C:4:GLU:HB2	1.85	0.41
2:B:28:PRO:CB	2:D:21:GLU:O	2.69	0.41
2:B:28:PRO:CG	2:D:23:GLY:N	2.75	0.41
1:C:21:ASN:OD1	2:D:23:GLY:C	2.60	0.40
2:D:1:PHE:CG	2:D:2:VAL:N	2.89	0.40

There are no symmetry-related clashes.

4.3 Torsion angles (i)

4.3.1 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	19/21 (90%)	18 (95%)	1 (5%)	0	100	100
1	C	19/21 (90%)	18 (95%)	1 (5%)	0	100	100
2	B	28/30 (93%)	26 (93%)	2 (7%)	0	100	100
2	D	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
All	All	94/102 (92%)	89 (95%)	5 (5%)	0	100	100

There are no Ramachandran outliers to report.

4.3.2 Protein sidechains (i)

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	20/20 (100%)	15 (75%)	5 (25%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	20/20 (100%)	15 (75%)	5 (25%)	0 0
2	B	26/26 (100%)	22 (85%)	4 (15%)	2 2
2	D	26/26 (100%)	19 (73%)	7 (27%)	0 0
All	All	92/92 (100%)	71 (77%)	21 (23%)	1 1

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	9	SER
1	A	11	CYS
1	A	12	SER
1	A	16	LEU
2	B	15	LEU
2	B	16	TYR
2	B	27	THR
2	B	30	THR
1	C	7	CYS
1	C	8	THR
1	C	9	SER
1	C	12	SER
1	C	14	TYR
2	D	1	PHE
2	D	4	GLN
2	D	7	CYS
2	D	12	VAL
2	D	16	TYR
2	D	27	THR
2	D	30	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
2	B	5	HIS
1	C	21	ASN
2	D	4	GLN

4.3.3 RNA

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.