



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:38 PM UTC

PDB ID : 2Q4C / pdb_00002q4c
Title : Ensemble refinement of the protein crystal structure of annexin from Arabidopsis thaliana gene At1g35720
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2007-05-31
Resolution : 2.51 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

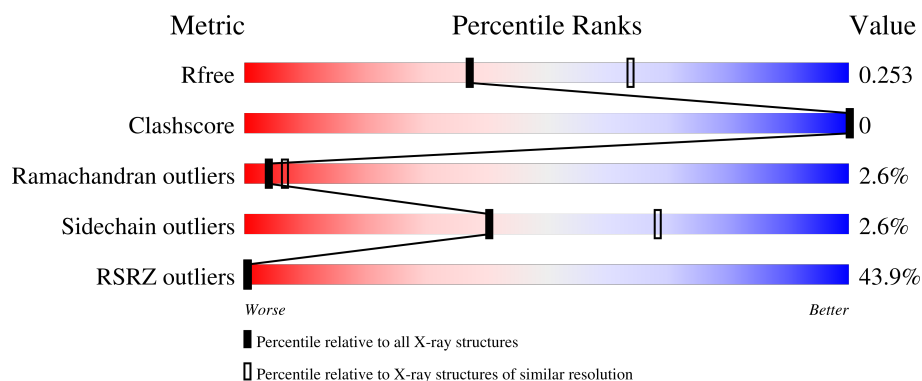
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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.



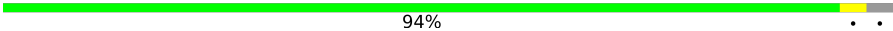
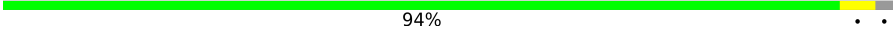
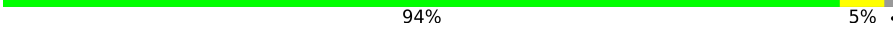
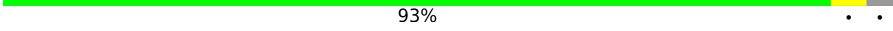
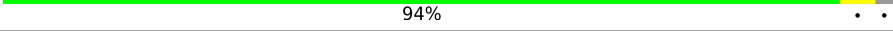
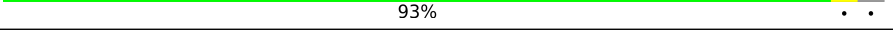
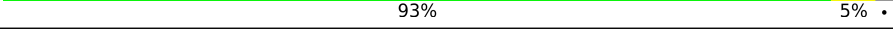
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	1-A	317	39% 94%
1	1-B	317	46% 92%
1	2-A	317	95%
1	2-B	317	93%
1	3-A	317	93% 5%

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Mol	Chain	Length	Quality of chain
1	3-B	317	 92% . . .
1	4-A	317	 91% 7% .
1	4-B	317	 94% . .
1	5-A	317	 94% . .
1	5-B	317	 92% . .
1	6-A	317	 94% 5% .
1	6-B	317	 93% . .
1	7-A	317	 94% . .
1	7-B	317	 93% . .
1	8-A	317	 93% 5% .
1	8-B	317	 91% 6% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 42008 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 Annexin D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	312	Total	C	N	O	S	0	0	0
			2508	1557	442	504	5			
1	2-A	312	Total	C	N	O	S	0	0	0
			2508	1557	442	504	5			
1	3-A	312	Total	C	N	O	S	0	0	0
			2508	1557	442	504	5			
1	4-A	312	Total	C	N	O	S	0	0	0
			2508	1557	442	504	5			
1	5-A	312	Total	C	N	O	S	0	0	0
			2508	1557	442	504	5			
1	6-A	312	Total	C	N	O	S	0	0	0
			2508	1557	442	504	5			
1	7-A	312	Total	C	N	O	S	0	0	0
			2508	1557	442	504	5			
1	8-A	312	Total	C	N	O	S	0	0	0
			2508	1557	442	504	5			
1	1-B	307	Total	C	N	O	S	0	0	0
			2462	1526	436	495	5			
1	2-B	307	Total	C	N	O	S	0	0	0
			2462	1526	436	495	5			
1	3-B	307	Total	C	N	O	S	0	0	0
			2462	1526	436	495	5			
1	4-B	307	Total	C	N	O	S	0	0	0
			2462	1526	436	495	5			
1	5-B	307	Total	C	N	O	S	0	0	0
			2462	1526	436	495	5			
1	6-B	307	Total	C	N	O	S	0	0	0
			2462	1526	436	495	5			
1	7-B	307	Total	C	N	O	S	0	0	0
			2462	1526	436	495	5			
1	8-B	307	Total	C	N	O	S	0	0	0
			2462	1526	436	495	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q9SYT0
B	1	SER	-	expression tag	UNP Q9SYT0

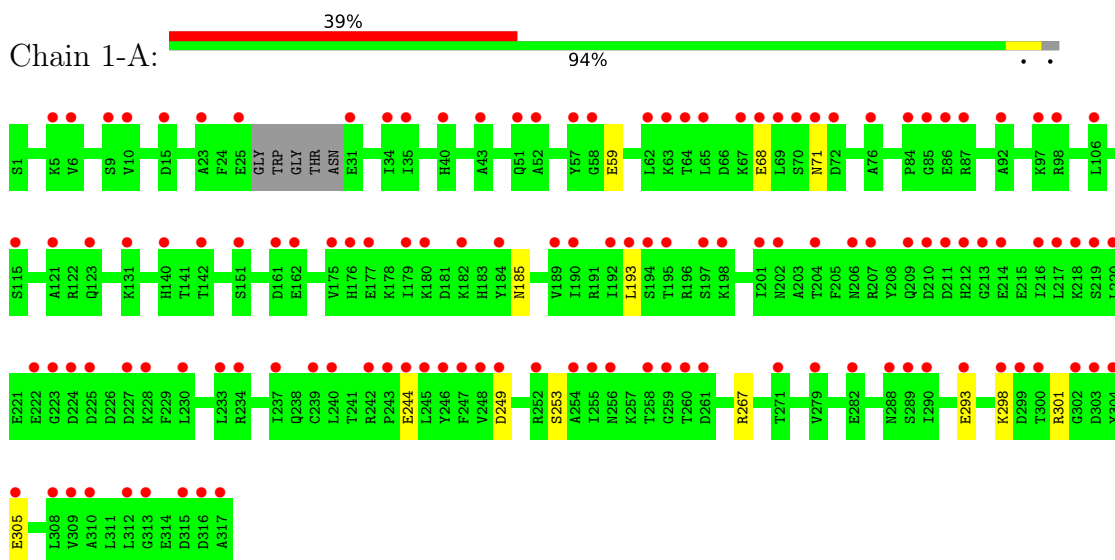
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1-A	170	Total	O	0	0
			170	170		
2	2-A	167	Total	O	0	0
			167	167		
2	3-A	164	Total	O	0	0
			164	164		
2	4-A	167	Total	O	0	0
			167	167		
2	5-A	171	Total	O	0	0
			171	171		
2	6-A	165	Total	O	0	0
			165	165		
2	7-A	165	Total	O	0	0
			165	165		
2	8-A	165	Total	O	0	0
			165	165		
2	1-B	111	Total	O	0	0
			111	111		
2	2-B	114	Total	O	0	0
			114	114		
2	3-B	117	Total	O	0	0
			117	117		
2	4-B	114	Total	O	0	0
			114	114		
2	5-B	110	Total	O	0	0
			110	110		
2	6-B	116	Total	O	0	0
			116	116		
2	7-B	116	Total	O	0	0
			116	116		
2	8-B	116	Total	O	0	0
			116	116		

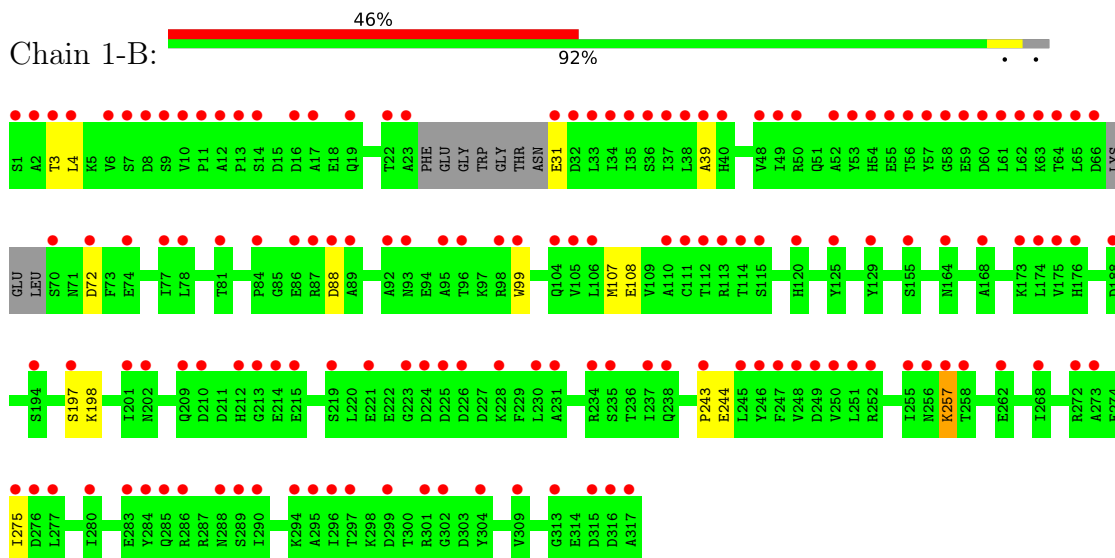
3 Residue-property plots

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: Annexin D1

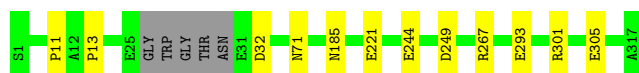


• Molecule 1: Annexin D1



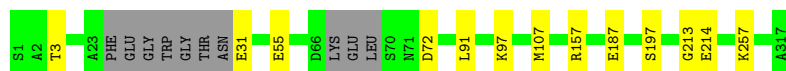
• Molecule 1: Annexin D1





- Molecule 1: Annexin D1

Chain 2-B: 93%



- Molecule 1: Annexin D1

Chain 3-A: 93% 5%



- Molecule 1: Annexin D1

Chain 3-B: 92%



- Molecule 1: Annexin D1

Chain 4-A: 91% 7%



- Molecule 1: Annexin D1

Chain 4-B: 94%



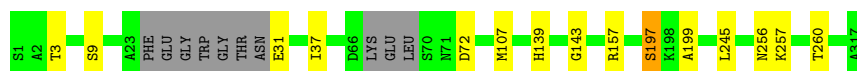
- Molecule 1: Annexin D1

Chain 5-A: 94%



- Molecule 1: Annexin D1

Chain 5-B: 92%



- Molecule 1: Annexin D1

Chain 6-A: 94% 5%



- Molecule 1: Annexin D1

Chain 6-B: 93% 5%



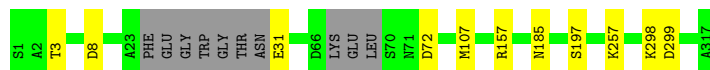
- Molecule 1: Annexin D1

Chain 7-A: 94% 5%



- Molecule 1: Annexin D1

Chain 7-B: 93% 5%



- Molecule 1: Annexin D1

Chain 8-A: 93% 5%



- Molecule 1: Annexin D1

Chain 8-B: 91% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	75.54Å 96.94Å 226.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.81 – 2.51 29.81 – 2.51	Depositor EDS
% Data completeness (in resolution range)	93.6 (29.81-2.51) 93.5 (29.81-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.79 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.177 , 0.243 0.188 , 0.253	Depositor DCC
R_{free} test set	1320 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.04 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	42008	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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](#)

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	1-A	0.20	0/2541	0.38	0/3428
1	1-B	0.18	0/2493	0.40	0/3363
1	2-A	0.20	0/2541	0.38	0/3428
1	2-B	0.18	0/2493	0.40	0/3363
1	3-A	0.20	0/2541	0.38	0/3428
1	3-B	0.18	0/2493	0.40	0/3363
1	4-A	0.20	0/2541	0.38	0/3428
1	4-B	0.18	0/2493	0.40	0/3363
1	5-A	0.20	0/2541	0.38	0/3428
1	5-B	0.18	0/2493	0.40	0/3363
1	6-A	0.20	0/2541	0.38	0/3428
1	6-B	0.18	0/2493	0.40	0/3363
1	7-A	0.20	0/2541	0.38	0/3428
1	7-B	0.18	0/2493	0.40	0/3363
1	8-A	0.20	0/2541	0.38	0/3428
1	8-B	0.18	0/2493	0.40	0/3363
All	All	0.19	0/40272	0.39	0/54328

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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	1-A	2508	0	2493	0	0
1	1-B	2462	0	2447	0	0
1	2-A	2508	0	2493	0	0
1	2-B	2462	0	2447	0	0
1	3-A	2508	0	2493	0	0
1	3-B	2462	0	2447	0	0
1	4-A	2508	0	2493	0	0
1	4-B	2462	0	2447	0	0
1	5-A	2508	0	2493	0	0
1	5-B	2462	0	2447	0	0
1	6-A	2508	0	2493	0	0
1	6-B	2462	0	2447	0	0
1	7-A	2508	0	2493	0	0
1	7-B	2462	0	2447	0	0
1	8-A	2508	0	2493	0	0
1	8-B	2462	0	2447	0	0
2	1-A	170	0	0	0	0
2	1-B	111	0	0	0	0
2	2-A	167	0	0	0	0
2	2-B	114	0	0	0	0
2	3-A	164	0	0	0	0
2	3-B	117	0	0	0	0
2	4-A	167	0	0	0	0
2	4-B	114	0	0	0	0
2	5-A	171	0	0	0	0
2	5-B	110	0	0	0	0
2	6-A	165	0	0	0	0
2	6-B	116	0	0	0	0
2	7-A	165	0	0	0	0
2	7-B	116	0	0	0	0
2	8-A	165	0	0	0	0
2	8-B	116	0	0	0	0
All	All	42008	0	39520	0	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 0.

There are no clashes within the asymmetric unit.

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	1-A	308/317 (97%)	268 (87%)	35 (11%)	5 (2%)	7	14
1	1-B	301/317 (95%)	249 (83%)	42 (14%)	10 (3%)	3	4
1	2-A	308/317 (97%)	266 (86%)	38 (12%)	4 (1%)	9	18
1	2-B	301/317 (95%)	248 (82%)	46 (15%)	7 (2%)	5	8
1	3-A	308/317 (97%)	267 (87%)	32 (10%)	9 (3%)	3	5
1	3-B	301/317 (95%)	241 (80%)	48 (16%)	12 (4%)	2	3
1	4-A	308/317 (97%)	254 (82%)	40 (13%)	14 (4%)	2	2
1	4-B	301/317 (95%)	258 (86%)	40 (13%)	3 (1%)	12	24
1	5-A	308/317 (97%)	262 (85%)	40 (13%)	6 (2%)	6	11
1	5-B	301/317 (95%)	253 (84%)	38 (13%)	10 (3%)	3	4
1	6-A	308/317 (97%)	271 (88%)	30 (10%)	7 (2%)	5	8
1	6-B	301/317 (95%)	266 (88%)	29 (10%)	6 (2%)	6	10
1	7-A	308/317 (97%)	256 (83%)	46 (15%)	6 (2%)	6	11
1	7-B	301/317 (95%)	257 (85%)	39 (13%)	5 (2%)	7	13
1	8-A	308/317 (97%)	263 (85%)	36 (12%)	9 (3%)	3	5
1	8-B	301/317 (95%)	249 (83%)	39 (13%)	13 (4%)	2	2
All	All	4872/5072 (96%)	4128 (85%)	618 (13%)	126 (3%)	4	7

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	298	LYS
1	1-B	88	ASP
1	1-B	108	GLU
1	2-A	13	PRO
1	2-B	97	LYS
1	2-B	187	GLU

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Mol	Chain	Res	Type
1	3-A	79	LEU
1	3-A	157	ARG
1	4-A	37	ILE
1	4-A	262	GLU
1	6-A	298	LYS
1	7-A	130	LYS
1	7-B	298	LYS
1	8-B	186	ASP
1	1-A	59	GLU
1	1-A	68	GLU
1	1-B	198	LYS
1	2-B	55	GLU
1	2-B	157	ARG
1	2-B	213	GLY
1	3-A	24	PHE
1	3-A	78	LEU
1	3-A	81	THR
1	3-B	143	GLY
1	3-B	160	GLY
1	3-B	261	ASP
1	4-A	24	PHE
1	4-A	298	LYS
1	4-B	161	ASP
1	5-A	209	GLN
1	5-B	143	GLY
1	5-B	260	THR
1	6-A	130	LYS
1	6-A	162	GLU
1	6-A	214	GLU
1	6-B	185	ASN
1	6-B	213	GLY
1	6-B	214	GLU
1	7-A	42	SER
1	7-A	159	GLU
1	7-A	162	GLU
1	8-A	139	HIS
1	8-A	289	SER
1	8-B	56	THR
1	8-B	134	GLU
1	8-B	135	GLU
1	8-B	299	ASP
1	1-B	243	PRO

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Mol	Chain	Res	Type
1	1-B	257	LYS
1	2-B	214	GLU
1	3-A	101	SER
1	3-A	197	SER
1	4-A	42	SER
1	4-A	160	GLY
1	5-A	286	ARG
1	5-B	9	SER
1	5-B	139	HIS
1	5-B	197	SER
1	5-B	199	ALA
1	6-A	213	GLY
1	7-A	24	PHE
1	7-B	8	ASP
1	7-B	299	ASP
1	8-A	143	GLY
1	8-A	257	LYS
1	8-A	277	LEU
1	8-B	131	LYS
1	8-B	282	GLU
1	8-B	298	LYS
1	8-B	301	ARG
1	1-A	193	LEU
1	1-A	253	SER
1	1-B	99	TRP
1	2-A	32	ASP
1	2-B	91	LEU
1	3-A	80	TRP
1	3-B	72	ASP
1	3-B	185	ASN
1	3-B	257	LYS
1	4-A	187	GLU
1	4-A	189	VAL
1	4-A	213	GLY
1	5-A	81	THR
1	5-A	257	LYS
1	5-A	262	GLU
1	5-B	157	ARG
1	5-B	245	LEU
1	5-B	256	ASN
1	6-A	8	ASP
1	7-B	157	ARG

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Mol	Chain	Res	Type
1	8-A	160	GLY
1	8-A	276	ASP
1	8-B	217	LEU
1	1-B	39	ALA
1	1-B	244	GLU
1	2-A	221	GLU
1	3-A	42	SER
1	3-B	105	VAL
1	3-B	126	HIS
1	3-B	301	ARG
1	4-A	133	LEU
1	4-A	143	GLY
1	4-A	214	GLU
1	4-A	216	ILE
1	4-B	221	GLU
1	7-A	160	GLY
1	7-B	185	ASN
1	8-B	149	LEU
1	8-B	150	VAL
1	1-B	4	LEU
1	5-A	315	ASP
1	6-A	143	GLY
1	6-B	79	LEU
1	6-B	191	ARG
1	8-B	112	THR
1	3-B	223	GLY
1	8-A	275	ILE
1	6-B	84	PRO
1	1-B	275	ILE
1	2-A	11	PRO
1	3-B	13	PRO
1	4-A	243	PRO
1	8-A	13	PRO
1	3-B	275	ILE
1	4-B	37	ILE
1	5-B	37	ILE

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	1-A	274/277 (99%)	266 (97%)	8 (3%)	37	65
1	1-B	269/277 (97%)	263 (98%)	6 (2%)	45	73
1	2-A	274/277 (99%)	266 (97%)	8 (3%)	37	65
1	2-B	269/277 (97%)	263 (98%)	6 (2%)	45	73
1	3-A	274/277 (99%)	266 (97%)	8 (3%)	37	65
1	3-B	269/277 (97%)	263 (98%)	6 (2%)	45	73
1	4-A	274/277 (99%)	266 (97%)	8 (3%)	37	65
1	4-B	269/277 (97%)	263 (98%)	6 (2%)	45	73
1	5-A	274/277 (99%)	266 (97%)	8 (3%)	37	65
1	5-B	269/277 (97%)	263 (98%)	6 (2%)	45	73
1	6-A	274/277 (99%)	266 (97%)	8 (3%)	37	65
1	6-B	269/277 (97%)	263 (98%)	6 (2%)	45	73
1	7-A	274/277 (99%)	266 (97%)	8 (3%)	37	65
1	7-B	269/277 (97%)	263 (98%)	6 (2%)	45	73
1	8-A	274/277 (99%)	266 (97%)	8 (3%)	37	65
1	8-B	269/277 (97%)	263 (98%)	6 (2%)	45	73
All	All	4344/4432 (98%)	4232 (97%)	112 (3%)	40	68

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	71	ASN
1	1-A	185	ASN
1	1-A	244	GLU
1	1-A	249	ASP
1	1-A	267	ARG
1	1-A	293	GLU
1	1-A	301	ARG
1	1-A	305	GLU
1	1-B	3	THR
1	1-B	31	GLU
1	1-B	72	ASP
1	1-B	107	MET
1	1-B	197	SER
1	1-B	257	LYS

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Mol	Chain	Res	Type
1	2-A	71	ASN
1	2-A	185	ASN
1	2-A	244	GLU
1	2-A	249	ASP
1	2-A	267	ARG
1	2-A	293	GLU
1	2-A	301	ARG
1	2-A	305	GLU
1	2-B	3	THR
1	2-B	31	GLU
1	2-B	72	ASP
1	2-B	107	MET
1	2-B	197	SER
1	2-B	257	LYS
1	3-A	71	ASN
1	3-A	185	ASN
1	3-A	244	GLU
1	3-A	249	ASP
1	3-A	267	ARG
1	3-A	293	GLU
1	3-A	301	ARG
1	3-A	305	GLU
1	3-B	3	THR
1	3-B	31	GLU
1	3-B	72	ASP
1	3-B	107	MET
1	3-B	197	SER
1	3-B	257	LYS
1	4-A	71	ASN
1	4-A	185	ASN
1	4-A	244	GLU
1	4-A	249	ASP
1	4-A	267	ARG
1	4-A	293	GLU
1	4-A	301	ARG
1	4-A	305	GLU
1	4-B	3	THR
1	4-B	31	GLU
1	4-B	72	ASP
1	4-B	107	MET
1	4-B	197	SER
1	4-B	257	LYS

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Mol	Chain	Res	Type
1	5-A	71	ASN
1	5-A	185	ASN
1	5-A	244	GLU
1	5-A	249	ASP
1	5-A	267	ARG
1	5-A	293	GLU
1	5-A	301	ARG
1	5-A	305	GLU
1	5-B	3	THR
1	5-B	31	GLU
1	5-B	72	ASP
1	5-B	107	MET
1	5-B	197	SER
1	5-B	257	LYS
1	6-A	71	ASN
1	6-A	185	ASN
1	6-A	244	GLU
1	6-A	249	ASP
1	6-A	267	ARG
1	6-A	293	GLU
1	6-A	301	ARG
1	6-A	305	GLU
1	6-B	3	THR
1	6-B	31	GLU
1	6-B	72	ASP
1	6-B	107	MET
1	6-B	197	SER
1	6-B	257	LYS
1	7-A	71	ASN
1	7-A	185	ASN
1	7-A	244	GLU
1	7-A	249	ASP
1	7-A	267	ARG
1	7-A	293	GLU
1	7-A	301	ARG
1	7-A	305	GLU
1	7-B	3	THR
1	7-B	31	GLU
1	7-B	72	ASP
1	7-B	107	MET
1	7-B	197	SER
1	7-B	257	LYS

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Mol	Chain	Res	Type
1	8-A	71	ASN
1	8-A	185	ASN
1	8-A	244	GLU
1	8-A	249	ASP
1	8-A	267	ARG
1	8-A	293	GLU
1	8-A	301	ARG
1	8-A	305	GLU
1	8-B	3	THR
1	8-B	31	GLU
1	8-B	72	ASP
1	8-B	107	MET
1	8-B	197	SER
1	8-B	257	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	51	GLN
1	1-A	71	ASN
1	1-A	170	GLN
1	1-A	185	ASN
1	1-A	202	ASN
1	1-A	209	GLN
1	1-A	256	ASN
1	1-A	285	GLN
1	1-B	104	GLN
1	1-B	120	HIS
1	1-B	170	GLN
1	1-B	202	ASN
1	1-B	212	HIS
1	1-B	238	GLN
1	2-A	40	HIS
1	2-A	104	GLN
1	2-A	170	GLN
1	2-A	185	ASN
1	2-A	209	GLN
1	2-A	285	GLN
1	2-A	288	ASN
1	2-B	117	GLN
1	2-B	202	ASN
1	2-B	256	ASN

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Mol	Chain	Res	Type
1	3-A	54	HIS
1	3-A	103	ASN
1	3-A	170	GLN
1	3-A	185	ASN
1	3-A	202	ASN
1	3-A	209	GLN
1	3-A	238	GLN
1	3-B	93	ASN
1	3-B	139	HIS
1	3-B	170	GLN
1	3-B	176	HIS
1	3-B	238	GLN
1	3-B	285	GLN
1	4-A	40	HIS
1	4-A	93	ASN
1	4-A	104	GLN
1	4-A	170	GLN
1	4-A	185	ASN
1	4-A	200	GLN
1	4-A	202	ASN
1	4-A	212	HIS
1	4-A	285	GLN
1	4-A	288	ASN
1	4-B	45	GLN
1	4-B	117	GLN
1	4-B	139	HIS
1	4-B	170	GLN
1	4-B	176	HIS
1	4-B	285	GLN
1	5-A	93	ASN
1	5-A	170	GLN
1	5-A	183	HIS
1	5-A	185	ASN
1	5-A	200	GLN
1	5-A	206	ASN
1	5-A	285	GLN
1	5-B	40	HIS
1	5-B	71	ASN
1	5-B	117	GLN
1	5-B	170	GLN
1	5-B	176	HIS
1	5-B	200	GLN

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Mol	Chain	Res	Type
1	5-B	238	GLN
1	6-A	51	GLN
1	6-A	93	ASN
1	6-A	170	GLN
1	6-A	176	HIS
1	6-A	185	ASN
1	6-A	285	GLN
1	6-B	93	ASN
1	6-B	176	HIS
1	6-B	212	HIS
1	7-A	40	HIS
1	7-A	71	ASN
1	7-A	120	HIS
1	7-A	123	GLN
1	7-A	140	HIS
1	7-A	170	GLN
1	7-A	176	HIS
1	7-A	185	ASN
1	7-A	206	ASN
1	7-A	209	GLN
1	7-A	212	HIS
1	7-A	238	GLN
1	7-A	256	ASN
1	7-A	285	GLN
1	7-B	19	GLN
1	7-B	104	GLN
1	7-B	176	HIS
1	7-B	202	ASN
1	7-B	285	GLN
1	8-A	117	GLN
1	8-A	140	HIS
1	8-A	170	GLN
1	8-A	185	ASN
1	8-A	202	ASN
1	8-A	206	ASN
1	8-A	256	ASN
1	8-A	285	GLN
1	8-B	19	GLN
1	8-B	51	GLN
1	8-B	170	GLN
1	8-B	176	HIS
1	8-B	202	ASN

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](#)

There are no ligands in this entry.

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

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	1-A	312/317 (98%)	2.01	125 (40%)  	1, 4, 8, 11	312 (100%)
1	1-B	307/317 (96%)	2.20	147 (47%)  	2, 5, 9, 11	307 (100%)
1	2-A	0/317	-	-	-	-
1	2-B	0/317	-	-	-	-
1	3-A	0/317	-	-	-	-
1	3-B	0/317	-	-	-	-
1	4-A	0/317	-	-	-	-
1	4-B	0/317	-	-	-	-
1	5-A	0/317	-	-	-	-
1	5-B	0/317	-	-	-	-
1	6-A	0/317	-	-	-	-
1	6-B	0/317	-	-	-	-
1	7-A	0/317	-	-	-	-
1	7-B	0/317	-	-	-	-
1	8-A	0/317	-	-	-	-
1	8-B	0/317	-	-	-	-
All	All	619/5072 (12%)	2.11	272 (43%)  	1, 4, 9, 11	619 (100%)

All (272) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	92	ALA	8.2
1	1-B	54	HIS	8.0
1	1-B	89	ALA	7.9
1	1-A	225	ASP	7.0
1	1-B	59	GLU	6.8
1	1-B	106	LEU	6.6
1	1-B	283	GLU	6.6
1	1-A	209	GLN	6.5
1	1-A	195	THR	6.3
1	1-B	289	SER	5.9

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Mol	Chain	Res	Type	RSRZ
1	1-A	213	GLY	5.9
1	1-A	223	GLY	5.7
1	1-A	69	LEU	5.7
1	1-B	65	LEU	5.6
1	1-A	220	LEU	5.5
1	1-B	7	SER	5.5
1	1-A	63	LYS	5.4
1	1-A	197	SER	5.4
1	1-B	3	THR	5.3
1	1-B	112	THR	5.3
1	1-A	303	ASP	5.3
1	1-B	155	SER	5.2
1	1-A	214	GLU	5.1
1	1-B	275	ILE	5.1
1	1-A	248	VAL	5.1
1	1-A	206	ASN	5.1
1	1-A	244	GLU	5.0
1	1-B	58	GLY	4.9
1	1-B	115	SER	4.8
1	1-B	2	ALA	4.7
1	1-B	49	ILE	4.7
1	1-B	290	ILE	4.6
1	1-B	62	LEU	4.6
1	1-B	57	TYR	4.6
1	1-B	273	ALA	4.5
1	1-A	300	THR	4.5
1	1-A	210	ASP	4.5
1	1-B	249	ASP	4.5
1	1-A	64	THR	4.4
1	1-A	290	ILE	4.4
1	1-A	245	LEU	4.4
1	1-B	247	PHE	4.4
1	1-B	317	ALA	4.4
1	1-B	280	ILE	4.3
1	1-A	71	ASN	4.3
1	1-B	14	SER	4.3
1	1-B	246	TYR	4.3
1	1-A	176	HIS	4.2
1	1-B	301	ARG	4.2
1	1-A	315	ASP	4.2
1	1-B	215	GLU	4.2
1	1-B	221	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	1-A	67	LYS	4.1
1	1-A	304	TYR	4.1
1	1-B	248	VAL	4.1
1	1-A	9	SER	4.0
1	1-B	64	THR	4.0
1	1-A	246	TYR	4.0
1	1-A	243	PRO	4.0
1	1-B	38	LEU	3.9
1	1-A	259	GLY	3.9
1	1-B	61	LEU	3.9
1	1-B	10	VAL	3.9
1	1-B	309	VAL	3.9
1	1-B	277	LEU	3.8
1	1-B	23	ALA	3.8
1	1-B	31	GLU	3.8
1	1-A	247	PHE	3.8
1	1-B	32	ASP	3.8
1	1-B	60	ASP	3.8
1	1-B	87	ARG	3.7
1	1-B	56	THR	3.7
1	1-B	93	ASN	3.7
1	1-B	276	ASP	3.7
1	1-A	224	ASP	3.6
1	1-A	184	TYR	3.6
1	1-B	250	VAL	3.6
1	1-A	62	LEU	3.6
1	1-B	4	LEU	3.6
1	1-A	10	VAL	3.6
1	1-B	202	ASN	3.6
1	1-A	305	GLU	3.6
1	1-B	262	GLU	3.6
1	1-B	50	ARG	3.6
1	1-B	243	PRO	3.6
1	1-A	211	ASP	3.6
1	1-A	25	GLU	3.5
1	1-A	239	CYS	3.5
1	1-A	15	ASP	3.5
1	1-B	234	ARG	3.5
1	1-A	240	LEU	3.4
1	1-A	293	GLU	3.4
1	1-B	256	ASN	3.3
1	1-B	48	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	1-A	302	GLY	3.3
1	1-A	192	ILE	3.3
1	1-A	204	THR	3.3
1	1-A	299	ASP	3.3
1	1-B	111	CYS	3.3
1	1-A	256	ASN	3.3
1	1-B	224	ASP	3.3
1	1-A	98	ARG	3.3
1	1-A	222	GLU	3.2
1	1-B	9	SER	3.2
1	1-B	81	THR	3.2
1	1-A	279	VAL	3.2
1	1-B	36	SER	3.1
1	1-B	294	LYS	3.1
1	1-A	65	LEU	3.1
1	1-B	268	ILE	3.1
1	1-A	233	LEU	3.1
1	1-A	34	ILE	3.1
1	1-B	258	THR	3.1
1	1-B	295	ALA	3.1
1	1-A	194	SER	3.1
1	1-A	261	ASP	3.1
1	1-A	313	GLY	3.1
1	1-A	189	VAL	3.1
1	1-B	105	VAL	3.1
1	1-A	260	THR	3.1
1	1-B	53	TYR	3.1
1	1-A	31	GLU	3.1
1	1-B	70	SER	3.1
1	1-B	237	ILE	3.1
1	1-A	51	GLN	3.0
1	1-A	212	HIS	3.0
1	1-B	213	GLY	3.0
1	1-B	99	TRP	3.0
1	1-A	242	ARG	3.0
1	1-A	131	LYS	3.0
1	1-A	230	LEU	3.0
1	1-B	88	ASP	3.0
1	1-A	312	LEU	2.9
1	1-B	302	GLY	2.9
1	1-A	237	ILE	2.9
1	1-B	297	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	1-B	52	ALA	2.9
1	1-B	174	LEU	2.9
1	1-B	238	GLN	2.9
1	1-B	1	SER	2.9
1	1-B	104	GLN	2.9
1	1-A	179	ILE	2.8
1	1-B	212	HIS	2.8
1	1-B	223	GLY	2.8
1	1-A	202	ASN	2.8
1	1-B	175	VAL	2.8
1	1-A	258	THR	2.8
1	1-B	214	GLU	2.8
1	1-B	188	ASP	2.8
1	1-B	37	ILE	2.8
1	1-B	66	ASP	2.8
1	1-B	129	TYR	2.7
1	1-B	114	THR	2.7
1	1-B	98	ARG	2.7
1	1-B	19	GLN	2.7
1	1-A	6	VAL	2.7
1	1-A	228	LYS	2.7
1	1-B	12	ALA	2.7
1	1-B	95	ALA	2.7
1	1-A	87	ARG	2.7
1	1-A	84	PRO	2.7
1	1-A	161	ASP	2.7
1	1-A	227	ASP	2.7
1	1-B	34	ILE	2.7
1	1-B	257	LYS	2.7
1	1-A	106	LEU	2.7
1	1-A	249	ASP	2.6
1	1-A	86	GLU	2.6
1	1-A	140	HIS	2.6
1	1-A	218	LYS	2.6
1	1-B	272	ARG	2.6
1	1-B	235	SER	2.6
1	1-B	316	ASP	2.6
1	1-A	123	GLN	2.6
1	1-B	55	GLU	2.6
1	1-A	310	ALA	2.6
1	1-B	284	TYR	2.6
1	1-B	16	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	1-B	35	ILE	2.5
1	1-B	6	VAL	2.5
1	1-A	198	LYS	2.5
1	1-A	255	ILE	2.5
1	1-A	162	GLU	2.5
1	1-A	309	VAL	2.5
1	1-B	72	ASP	2.5
1	1-B	86	GLU	2.5
1	1-B	120	HIS	2.5
1	1-A	43	ALA	2.5
1	1-A	35	ILE	2.5
1	1-A	316	ASP	2.5
1	1-B	285	GLN	2.5
1	1-B	286	ARG	2.5
1	1-B	17	ALA	2.5
1	1-A	115	SER	2.5
1	1-A	271	THR	2.5
1	1-B	245	LEU	2.4
1	1-A	177	GLU	2.4
1	1-A	58	GLY	2.4
1	1-A	40	HIS	2.4
1	1-B	113	ARG	2.4
1	1-A	142	THR	2.4
1	1-B	194	SER	2.4
1	1-A	52	ALA	2.4
1	1-B	74	GLU	2.4
1	1-B	313	GLY	2.3
1	1-A	207	ARG	2.3
1	1-A	216	ILE	2.3
1	1-A	252	ARG	2.3
1	1-A	308	LEU	2.3
1	1-B	210	ASP	2.3
1	1-B	96	THR	2.3
1	1-B	77	ILE	2.3
1	1-B	176	HIS	2.3
1	1-B	209	GLN	2.3
1	1-B	255	ILE	2.3
1	1-B	8	ASP	2.3
1	1-A	182	LYS	2.3
1	1-B	63	LYS	2.3
1	1-A	57	TYR	2.3
1	1-A	234	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	1-A	201	ILE	2.3
1	1-B	201	ILE	2.3
1	1-A	5	LYS	2.3
1	1-B	304	TYR	2.3
1	1-B	230	LEU	2.2
1	1-B	296	ILE	2.2
1	1-B	11	PRO	2.2
1	1-A	254	ALA	2.2
1	1-A	288	ASN	2.2
1	1-B	39	ALA	2.2
1	1-B	288	ASN	2.2
1	1-A	72	ASP	2.2
1	1-B	299	ASP	2.2
1	1-B	110	ALA	2.2
1	1-B	173	LYS	2.2
1	1-A	175	VAL	2.2
1	1-A	70	SER	2.2
1	1-B	219	SER	2.2
1	1-B	225	ASP	2.2
1	1-B	226	ASP	2.2
1	1-B	84	PRO	2.2
1	1-A	180	LYS	2.2
1	1-B	40	HIS	2.1
1	1-B	168	ALA	2.1
1	1-A	282	GLU	2.1
1	1-B	197	SER	2.1
1	1-B	13	PRO	2.1
1	1-B	228	LYS	2.1
1	1-A	317	ALA	2.1
1	1-A	85	GLY	2.1
1	1-A	193	LEU	2.1
1	1-A	217	LEU	2.1
1	1-A	190	ILE	2.1
1	1-B	33	LEU	2.1
1	1-B	78	LEU	2.1
1	1-A	151	SER	2.1
1	1-B	92	ALA	2.1
1	1-B	164	ASN	2.1
1	1-B	252	ARG	2.1
1	1-A	97	LYS	2.1
1	1-A	298	LYS	2.1
1	1-B	315	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	1-A	76	ALA	2.0
1	1-A	121	ALA	2.0
1	1-A	68	GLU	2.0
1	1-B	22	THR	2.0
1	1-B	125	TYR	2.0
1	1-A	219	SER	2.0
1	1-A	23	ALA	2.0
1	1-B	231	ALA	2.0
1	1-B	251	LEU	2.0
1	1-A	289	SER	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.