



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 08:37 AM UTC

PDB ID : 2BDI / pdb_00002bdi
Title : Human Kallikrein 4 complex with cobalt and p-aminobenzamidine
Authors : Debela, M.; Bode, W.; Goettig, P.; Structural Proteomics in Europe (SPINE)
Deposited on : 2005-10-20
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

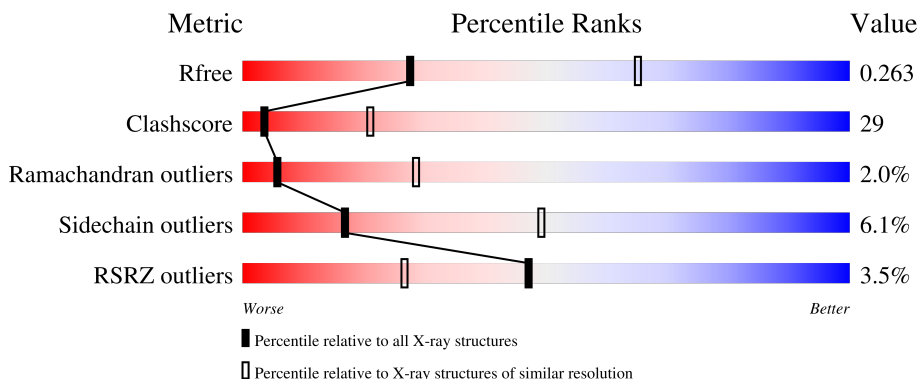
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.



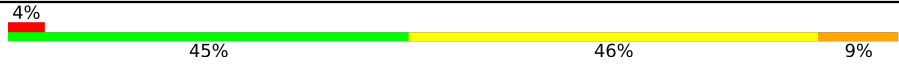



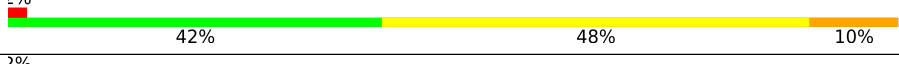
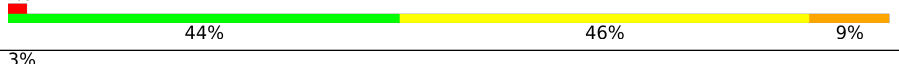
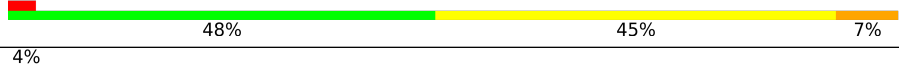
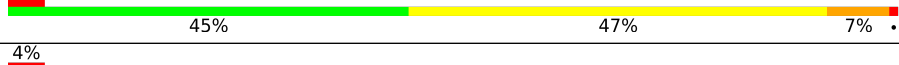
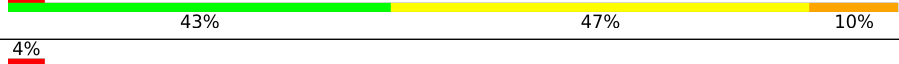
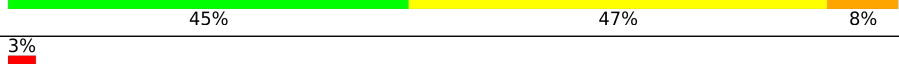

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	223	
1	B	223	
1	C	223	
1	D	223	
1	E	223	

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Mol	Chain	Length	Quality of chain
1	F	223	
1	G	223	
1	H	223	
1	I	223	
1	J	223	
1	K	223	
1	L	223	
1	M	223	
1	N	223	
1	O	223	
1	P	223	

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
3	PBZ	A	701	-	X	-	-
3	PBZ	D	704	-	-	X	-
3	PBZ	L	712	-	X	-	-
3	PBZ	O	715	-	X	X	-
3	PBZ	P	716	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 27340 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.

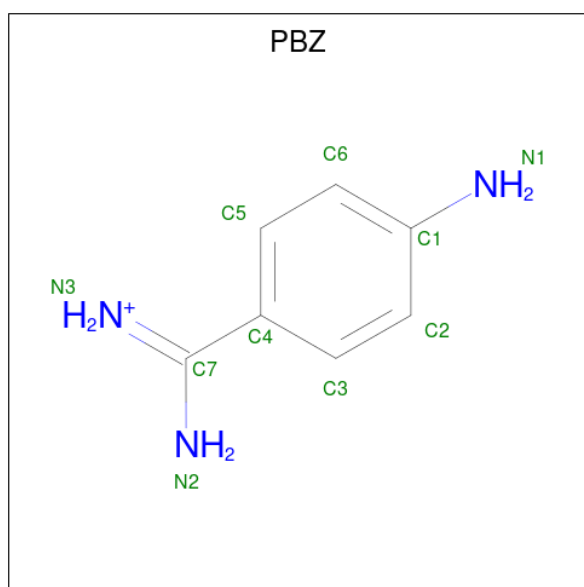
- Molecule 1 is a protein called Kallikrein-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	223	1670	1043	281	329	17	135	0	0
1	B	223	1670	1043	281	329	17	80	0	0
1	C	223	1670	1043	281	329	17	62	0	0
1	D	223	1670	1043	281	329	17	91	0	0
1	E	223	1670	1043	281	329	17	90	0	0
1	F	223	1670	1043	281	329	17	54	0	0
1	G	223	1670	1043	281	329	17	81	0	0
1	H	223	1670	1043	281	329	17	120	0	0
1	I	223	1670	1043	281	329	17	105	0	0
1	J	223	1670	1043	281	329	17	56	0	0
1	K	223	1670	1043	281	329	17	78	0	0
1	L	223	1670	1043	281	329	17	73	0	0
1	M	223	1670	1043	281	329	17	48	0	0
1	N	223	1670	1043	281	329	17	63	0	0
1	O	223	1670	1043	281	329	17	67	0	0
1	P	223	1670	1043	281	329	17	86	0	0

- Molecule 2 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Co 1 1	0	0
2	E	1	Total Co 1 1	0	0
2	I	1	Total Co 1 1	0	0
2	M	1	Total Co 1 1	0	0

- Molecule 3 is P-AMINO BENZAMIDINE (CCD ID: PBZ) (formula: C₇H₁₀N₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 10 7 3	0	0
3	B	1	Total C N 10 7 3	0	0
3	C	1	Total C N 10 7 3	0	0
3	D	1	Total C N 10 7 3	0	0
3	E	1	Total C N 10 7 3	0	0
3	F	1	Total C N 10 7 3	0	0
3	G	1	Total C N 10 7 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	N	0	0
			10	7	3		
3	I	1	Total	C	N	0	0
			10	7	3		
3	J	1	Total	C	N	0	0
			10	7	3		
3	K	1	Total	C	N	0	0
			10	7	3		
3	L	1	Total	C	N	0	0
			10	7	3		
3	M	1	Total	C	N	0	0
			10	7	3		
3	N	1	Total	C	N	0	0
			10	7	3		
3	O	1	Total	C	N	0	0
			10	7	3		
3	P	1	Total	C	N	0	0
			10	7	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total	O	0	0
			26	26		
4	B	27	Total	O	0	0
			27	27		
4	C	30	Total	O	0	0
			30	30		
4	D	37	Total	O	0	0
			37	37		
4	E	26	Total	O	0	0
			26	26		
4	F	36	Total	O	0	0
			36	36		
4	G	25	Total	O	0	0
			25	25		
4	H	21	Total	O	0	0
			21	21		
4	I	20	Total	O	0	0
			20	20		
4	J	22	Total	O	0	0
			22	22		

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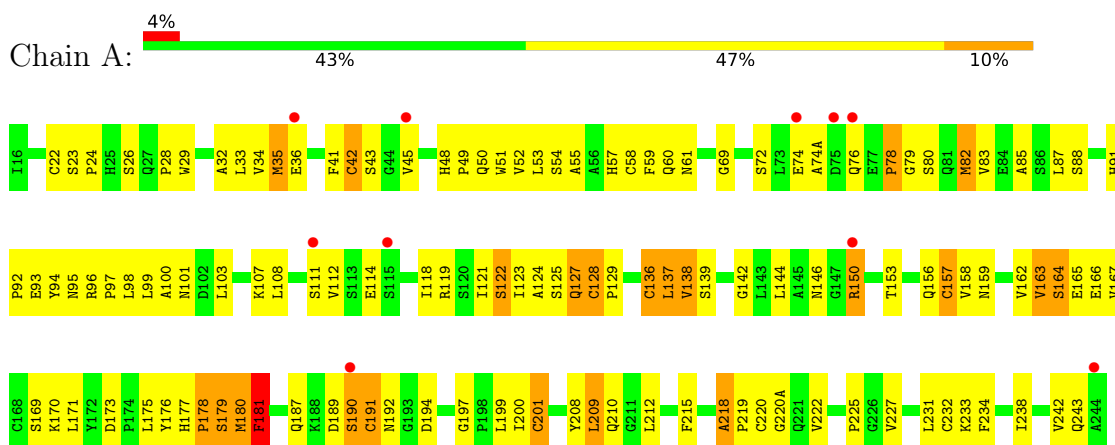
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	K	21	Total O 21 21	0	0
4	L	39	Total O 39 39	0	0
4	M	37	Total O 37 37	0	0
4	N	29	Total O 29 29	0	0
4	O	28	Total O 28 28	0	0
4	P	32	Total O 32 32	0	0

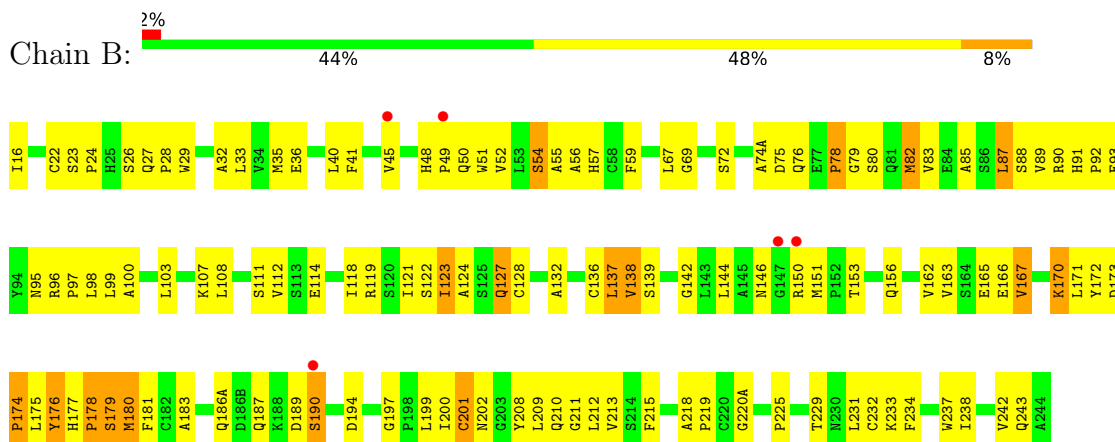
3 Residue-property plots

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.

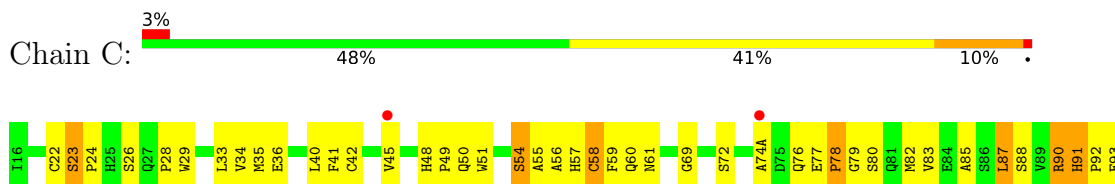
- Molecule 1: Kallikrein-4



- Molecule 1: Kallikrein-4

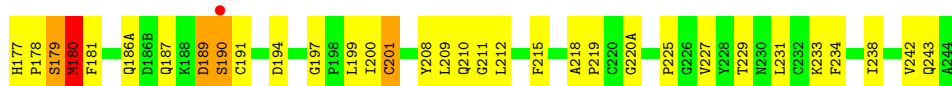
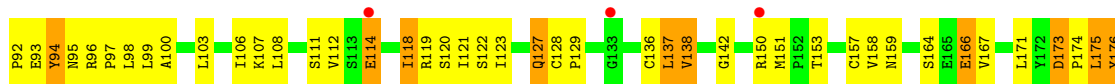
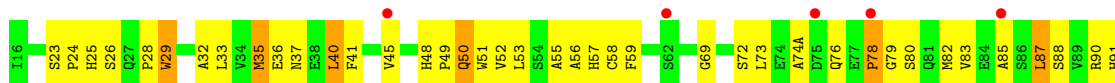


- Molecule 1: Kallikrein-4

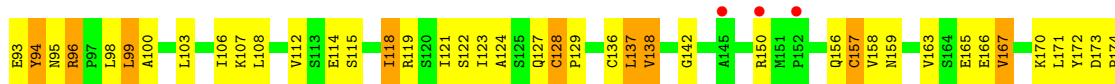
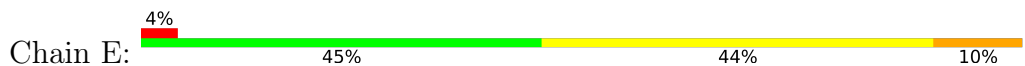




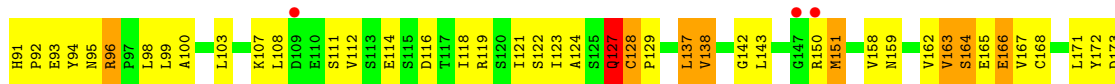
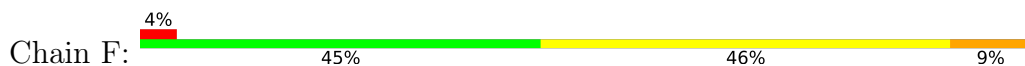
• Molecule 1: Kallikrein-4



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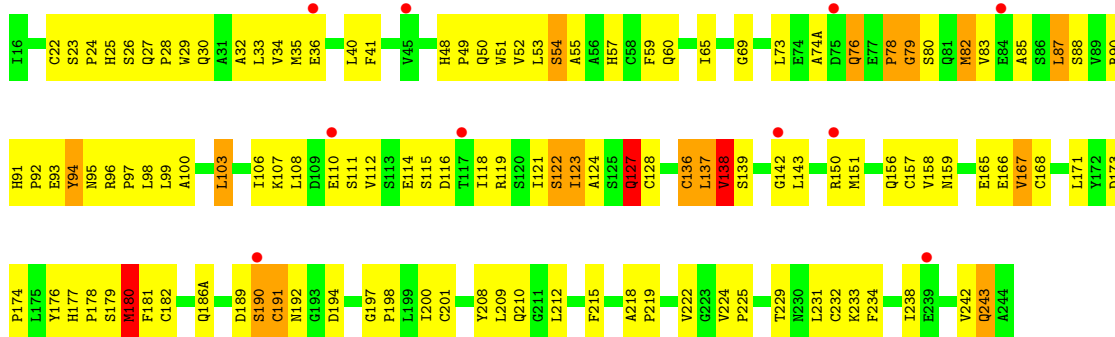


• Molecule 1: Kallikrein-4



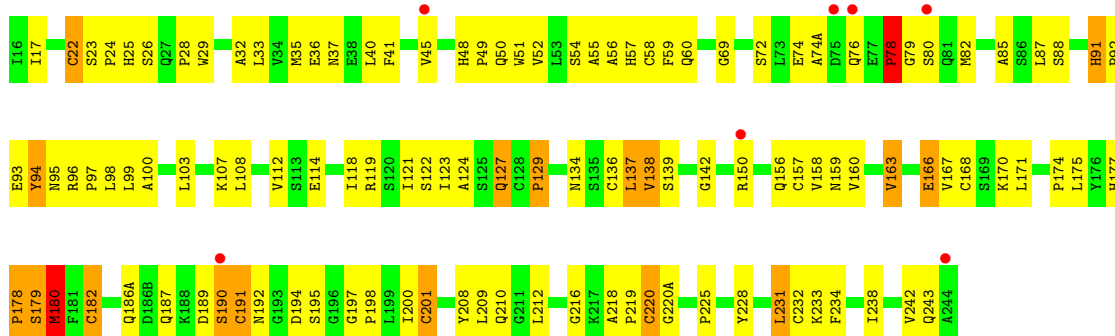
- Molecule 1: Kallikrein-4

Chain G: 4% 45% 47% 7%



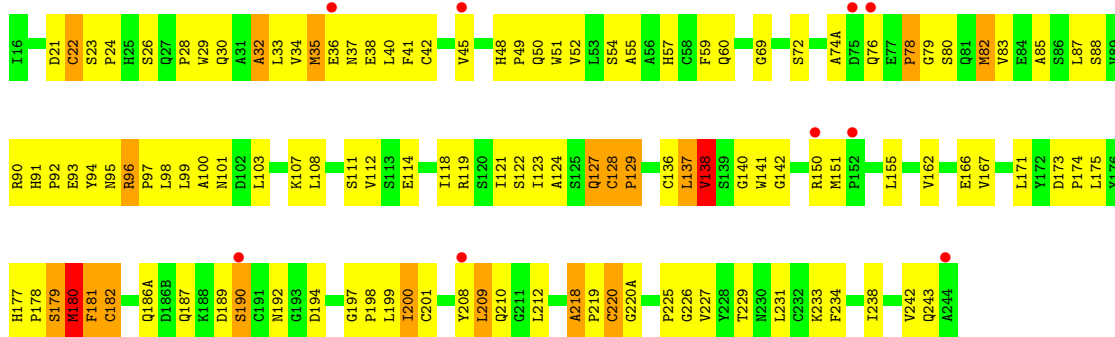
- Molecule 1: Kallikrein-4

Chain H: 3% 47% 44% 8%



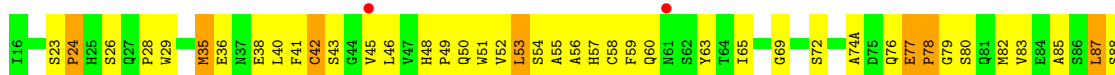
- Molecule 1: Kallikrein-4

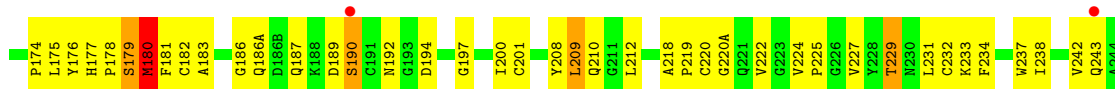
Chain I: 4% 47% 44% 8%



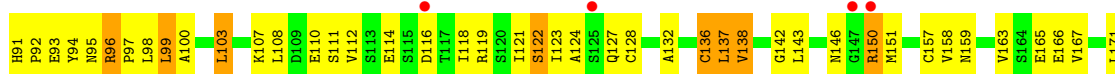
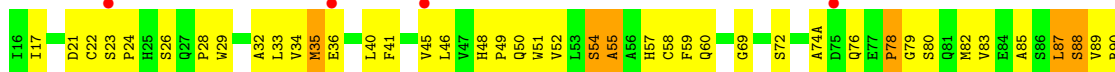
- Molecule 1: Kallikrein-4

Chain J: 2% 42% 48% 10%

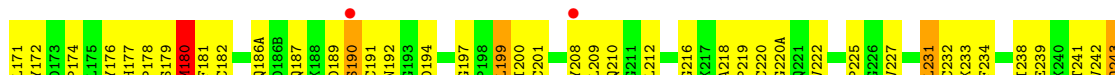




• Molecule 1: Kallikrein-4

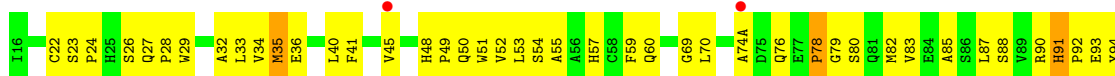


• Molecule 1: Kallikrein-4



A244

• Molecule 1: Kallikrein-4



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	147.05Å 73.86Å 154.38Å 90.00° 102.41° 90.00°	Depositor
Resolution (Å)	19.90 – 3.00 19.90 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.6 (19.90-3.00) 96.2 (19.90-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.98Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.258 , 0.296 0.259 , 0.263	Depositor DCC
R_{free} test set	3199 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtrriage
Anisotropy	0.279	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 62.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.000 for l,-k,h	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	27340	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.08 % 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 1.2048e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PBZ, CO

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	1.73	20/1707 (1.2%)	1.40	10/2323 (0.4%)
1	B	1.74	26/1707 (1.5%)	1.38	6/2323 (0.3%)
1	C	1.68	20/1707 (1.2%)	1.38	10/2323 (0.4%)
1	D	1.76	26/1707 (1.5%)	1.38	7/2323 (0.3%)
1	E	1.77	27/1707 (1.6%)	1.40	12/2323 (0.5%)
1	F	1.88	26/1707 (1.5%)	1.39	12/2323 (0.5%)
1	G	1.79	24/1707 (1.4%)	1.41	12/2323 (0.5%)
1	H	1.72	23/1707 (1.3%)	1.43	14/2323 (0.6%)
1	I	1.70	21/1707 (1.2%)	1.39	8/2323 (0.3%)
1	J	1.75	29/1707 (1.7%)	1.39	10/2323 (0.4%)
1	K	1.71	27/1707 (1.6%)	1.39	9/2323 (0.4%)
1	L	1.69	19/1707 (1.1%)	1.34	3/2323 (0.1%)
1	M	1.84	27/1707 (1.6%)	1.37	8/2323 (0.3%)
1	N	1.80	28/1707 (1.6%)	1.40	14/2323 (0.6%)
1	O	1.70	25/1707 (1.5%)	1.36	12/2323 (0.5%)
1	P	1.76	28/1707 (1.6%)	1.40	11/2323 (0.5%)
All	All	1.75	396/27312 (1.4%)	1.39	158/37168 (0.4%)

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
1	A	0	1
1	B	0	1
1	G	0	1
1	I	0	1
1	K	0	1
1	N	0	1
1	P	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	7

The worst 5 of 396 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	22	CYS	CA-C	12.87	1.69	1.52
1	L	201	CYS	CA-C	-11.14	1.41	1.53
1	G	180	MET	SD-CE	-9.48	1.55	1.79
1	C	191	CYS	C-O	-9.05	1.12	1.23
1	G	168	CYS	C-O	-9.04	1.13	1.24

The worst 5 of 158 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	128	CYS	N-CA-C	10.03	123.93	110.08
1	M	128	CYS	CA-C-N	8.79	128.87	119.90
1	M	128	CYS	C-N-CA	8.79	128.87	119.90
1	P	157	CYS	CA-CB-SG	-8.34	95.21	114.40
1	A	76	GLN	N-CA-C	-8.18	102.06	114.16

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	181	PHE	Sidechain
1	B	176	TYR	Sidechain
1	G	181	PHE	Sidechain
1	I	181	PHE	Sidechain
1	K	176	TYR	Sidechain

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	A	1670	0	1598	97	0
1	B	1670	0	1598	93	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1670	0	1598	99	3
1	D	1670	0	1598	93	0
1	E	1670	0	1600	88	1
1	F	1670	0	1598	94	1
1	G	1670	0	1602	125	1
1	H	1670	0	1598	83	2
1	I	1670	0	1598	90	1
1	J	1670	0	1598	103	0
1	K	1670	0	1598	96	0
1	L	1670	0	1598	90	0
1	M	1670	0	1598	89	0
1	N	1670	0	1600	100	1
1	O	1670	0	1598	90	1
1	P	1670	0	1598	103	0
2	A	1	0	0	0	0
2	E	1	0	0	0	0
2	I	1	0	0	0	0
2	M	1	0	0	0	0
3	A	10	0	10	2	0
3	B	10	0	10	2	0
3	C	10	0	10	0	0
3	D	10	0	10	7	0
3	E	10	0	10	2	0
3	F	10	0	10	1	0
3	G	10	0	10	2	0
3	H	10	0	8	5	0
3	I	10	0	10	2	0
3	J	10	0	10	2	0
3	K	10	0	10	0	0
3	L	10	0	10	1	0
3	M	10	0	10	2	0
3	N	10	0	10	2	0
3	O	10	0	10	8	0
3	P	10	0	10	6	0
4	A	26	0	0	7	0
4	B	27	0	0	5	0
4	C	30	0	0	3	1
4	D	37	0	0	6	0
4	E	26	0	0	6	0
4	F	36	0	0	8	1
4	G	25	0	0	11	0
4	H	21	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	20	0	0	7	0
4	J	22	0	0	6	0
4	K	21	0	0	2	1
4	L	39	0	0	8	1
4	M	37	0	0	5	0
4	N	29	0	0	6	0
4	O	28	0	0	1	0
4	P	32	0	0	15	0
All	All	27340	0	25734	1464	9

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 29.

The worst 5 of 1464 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:J:110:GLU:HA	4:J:731:HOH:O	1.31	1.21
1:B:136:CYS:HB3	1:B:200:ILE:O	1.40	1.20
1:I:96:ARG:NH1	4:I:719:HOH:O	1.91	1.02
1:G:116:ASP:HA	4:G:724:HOH:O	1.59	1.02
1:G:243:GLN:HG2	1:K:243:GLN:HB3	1.39	1.01

The worst 5 of 9 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:119:ARG:NH1	4:F:731:HOH:O[1_565]	1.91	0.29
1:E:84:GLU:OE2	1:G:76:GLN:OE1[2_555]	2.01	0.19
1:B:75:ASP:O	1:C:146:ASN:CB[2_544]	2.02	0.18
1:I:37:ASN:OD1	4:K:720:HOH:O[2_454]	2.09	0.11
1:N:239:GLU:CG	4:L:740:HOH:O[1_545]	2.09	0.11

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	221/223 (99%)	194 (88%)	22 (10%)	5 (2%)	5	25
1	B	221/223 (99%)	195 (88%)	22 (10%)	4 (2%)	6	31
1	C	221/223 (99%)	192 (87%)	25 (11%)	4 (2%)	6	31
1	D	221/223 (99%)	196 (89%)	21 (10%)	4 (2%)	6	31
1	E	221/223 (99%)	195 (88%)	22 (10%)	4 (2%)	6	31
1	F	221/223 (99%)	198 (90%)	19 (9%)	4 (2%)	6	31
1	G	221/223 (99%)	193 (87%)	24 (11%)	4 (2%)	6	31
1	H	221/223 (99%)	196 (89%)	19 (9%)	6 (3%)	4	22
1	I	221/223 (99%)	196 (89%)	20 (9%)	5 (2%)	5	25
1	J	221/223 (99%)	195 (88%)	22 (10%)	4 (2%)	6	31
1	K	221/223 (99%)	194 (88%)	23 (10%)	4 (2%)	6	31
1	L	221/223 (99%)	194 (88%)	22 (10%)	5 (2%)	5	25
1	M	221/223 (99%)	194 (88%)	23 (10%)	4 (2%)	6	31
1	N	221/223 (99%)	195 (88%)	22 (10%)	4 (2%)	6	31
1	O	221/223 (99%)	194 (88%)	22 (10%)	5 (2%)	5	25
1	P	221/223 (99%)	194 (88%)	23 (10%)	4 (2%)	6	31
All	All	3536/3568 (99%)	3115 (88%)	351 (10%)	70 (2%)	6	28

5 of 70 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	PRO
1	B	78	PRO
1	C	78	PRO
1	D	78	PRO
1	E	78	PRO

5.3.2 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	189/189 (100%)	177 (94%)	12 (6%)	16	48
1	B	189/189 (100%)	177 (94%)	12 (6%)	16	48
1	C	189/189 (100%)	175 (93%)	14 (7%)	13	42
1	D	189/189 (100%)	177 (94%)	12 (6%)	16	48
1	E	189/189 (100%)	178 (94%)	11 (6%)	18	51
1	F	189/189 (100%)	178 (94%)	11 (6%)	18	51
1	G	189/189 (100%)	179 (95%)	10 (5%)	20	54
1	H	189/189 (100%)	177 (94%)	12 (6%)	16	48
1	I	189/189 (100%)	179 (95%)	10 (5%)	20	54
1	J	189/189 (100%)	178 (94%)	11 (6%)	18	51
1	K	189/189 (100%)	177 (94%)	12 (6%)	16	48
1	L	189/189 (100%)	177 (94%)	12 (6%)	16	48
1	M	189/189 (100%)	177 (94%)	12 (6%)	16	48
1	N	189/189 (100%)	178 (94%)	11 (6%)	18	51
1	O	189/189 (100%)	178 (94%)	11 (6%)	18	51
1	P	189/189 (100%)	179 (95%)	10 (5%)	20	54
All	All	3024/3024 (100%)	2841 (94%)	183 (6%)	17	49

5 of 183 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	87	LEU
1	M	122	SER
1	K	137	LEU
1	L	127	GLN
1	M	190	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 142 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	101	ASN
1	M	221	GLN
1	O	50	GLN
1	F	18	ASN
1	E	221	GLN

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 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	PBZ	G	707	-	10,10,10	2.76	4 (40%)	9,13,13	1.76	3 (33%)
3	PBZ	C	703	-	10,10,10	2.15	4 (40%)	9,13,13	1.81	4 (44%)
3	PBZ	I	709	-	10,10,10	3.66	7 (70%)	9,13,13	0.85	0
3	PBZ	J	710	-	10,10,10	1.96	3 (30%)	9,13,13	1.12	1 (11%)
3	PBZ	K	711	-	10,10,10	2.09	2 (20%)	9,13,13	1.44	1 (11%)
3	PBZ	H	708	-	10,10,10	3.04	6 (60%)	9,13,13	1.43	0
3	PBZ	B	702	-	10,10,10	3.14	4 (40%)	9,13,13	1.44	1 (11%)
3	PBZ	D	704	-	10,10,10	2.34	3 (30%)	9,13,13	1.36	1 (11%)
3	PBZ	E	705	-	10,10,10	3.41	6 (60%)	9,13,13	1.40	1 (11%)
3	PBZ	L	712	-	10,10,10	3.73	9 (90%)	9,13,13	0.82	0
3	PBZ	P	716	-	10,10,10	3.71	8 (80%)	9,13,13	1.12	1 (11%)
3	PBZ	O	715	-	10,10,10	2.50	5 (50%)	9,13,13	2.11	5 (55%)
3	PBZ	A	701	-	10,10,10	4.46	7 (70%)	9,13,13	2.72	5 (55%)
3	PBZ	N	714	-	10,10,10	3.55	5 (50%)	9,13,13	2.04	3 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PBZ	F	706	-	10,10,10	1.70	2 (20%)	9,13,13	1.89	3 (33%)
3	PBZ	M	713	-	10,10,10	1.72	2 (20%)	9,13,13	1.88	3 (33%)

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	PBZ	G	707	-	-	2/4/4/4	0/1/1/1
3	PBZ	C	703	-	-	0/4/4/4	0/1/1/1
3	PBZ	I	709	-	-	2/4/4/4	0/1/1/1
3	PBZ	J	710	-	-	1/4/4/4	0/1/1/1
3	PBZ	K	711	-	-	2/4/4/4	0/1/1/1
3	PBZ	H	708	-	-	2/4/4/4	0/1/1/1
3	PBZ	B	702	-	-	2/4/4/4	0/1/1/1
3	PBZ	D	704	-	-	3/4/4/4	0/1/1/1
3	PBZ	E	705	-	-	0/4/4/4	0/1/1/1
3	PBZ	L	712	-	-	4/4/4/4	0/1/1/1
3	PBZ	P	716	-	-	2/4/4/4	0/1/1/1
3	PBZ	O	715	-	-	4/4/4/4	0/1/1/1
3	PBZ	A	701	-	-	3/4/4/4	0/1/1/1
3	PBZ	N	714	-	-	0/4/4/4	0/1/1/1
3	PBZ	F	706	-	-	4/4/4/4	0/1/1/1
3	PBZ	M	713	-	-	0/4/4/4	0/1/1/1

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	PBZ	C4-C7	8.97	1.64	1.47
3	A	701	PBZ	C5-C4	7.74	1.51	1.39
3	B	702	PBZ	C5-C4	7.04	1.50	1.39
3	L	712	PBZ	C4-C7	6.67	1.59	1.47
3	E	705	PBZ	C4-C7	6.48	1.59	1.47

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	PBZ	C2-C1-N1	-4.85	111.97	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	PBZ	C5-C6-C1	-4.36	115.34	120.66
3	F	706	PBZ	C2-C3-C4	-3.88	116.66	120.80
3	N	714	PBZ	C6-C5-C4	-3.73	116.82	120.80
3	O	715	PBZ	C6-C5-C4	3.66	124.71	120.80

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	704	PBZ	C3-C4-C7-N2
3	D	704	PBZ	C5-C4-C7-N2
3	H	708	PBZ	C3-C4-C7-N2
3	H	708	PBZ	C5-C4-C7-N2
3	K	711	PBZ	C3-C4-C7-N2

There are no ring outliers.

14 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	707	PBZ	2	0
3	I	709	PBZ	2	0
3	J	710	PBZ	2	0
3	H	708	PBZ	5	0
3	B	702	PBZ	2	0
3	D	704	PBZ	7	0
3	E	705	PBZ	2	0
3	L	712	PBZ	1	0
3	P	716	PBZ	6	0
3	O	715	PBZ	8	0
3	A	701	PBZ	2	0
3	N	714	PBZ	2	0
3	F	706	PBZ	1	0
3	M	713	PBZ	2	0

5.7 Other polymers [i](#)

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 [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	220/223 (98%)	0.38	10 (4%) 38 20	9, 30, 54, 68	28 (12%)
1	B	222/223 (99%)	0.29	5 (2%) 61 38	7, 28, 51, 65	20 (9%)
1	C	223/223 (100%)	0.31	7 (3%) 51 30	7, 28, 54, 66	18 (8%)
1	D	222/223 (99%)	0.32	9 (4%) 41 23	6, 28, 53, 67	22 (9%)
1	E	223/223 (100%)	0.27	8 (3%) 46 26	7, 26, 52, 65	24 (10%)
1	F	223/223 (100%)	0.30	10 (4%) 38 20	4, 26, 51, 64	17 (7%)
1	G	223/223 (100%)	0.47	10 (4%) 38 20	5, 29, 54, 64	20 (8%)
1	H	223/223 (100%)	0.32	7 (3%) 51 30	9, 27, 53, 68	30 (13%)
1	I	223/223 (100%)	0.44	9 (4%) 42 23	10, 29, 50, 64	30 (13%)
1	J	223/223 (100%)	0.33	4 (1%) 67 44	7, 30, 53, 64	18 (8%)
1	K	222/223 (99%)	0.36	5 (2%) 61 38	5, 28, 54, 63	22 (9%)
1	L	223/223 (100%)	0.26	7 (3%) 51 30	5, 30, 54, 67	20 (8%)
1	M	223/223 (100%)	0.28	10 (4%) 38 20	5, 26, 50, 62	16 (7%)
1	N	223/223 (100%)	0.28	10 (4%) 38 20	4, 27, 54, 68	18 (8%)
1	O	223/223 (100%)	0.28	8 (3%) 46 26	6, 26, 52, 63	19 (8%)
1	P	223/223 (100%)	0.34	7 (3%) 51 30	8, 29, 53, 65	23 (10%)
All	All	3562/3568 (99%)	0.33	126 (3%) 47 27	4, 28, 54, 68	345 (9%)

The worst 5 of 126 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	190	SER	7.2
1	I	190	SER	7.1
1	M	190	SER	6.7
1	K	190	SER	6.7
1	A	190	SER	6.7

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(\AA^2)	Q<0.9
2	CO	A	1	1/1	0.75	0.10	62,62,62,62	0
3	PBZ	G	707	10/10	0.77	0.22	62,65,66,67	0
3	PBZ	C	703	10/10	0.83	0.15	34,39,41,42	0
3	PBZ	N	714	10/10	0.84	0.15	33,39,41,45	0
3	PBZ	H	708	10/10	0.85	0.14	27,31,34,36	0
3	PBZ	L	712	10/10	0.86	0.13	35,37,42,45	0
3	PBZ	M	713	10/10	0.86	0.13	24,26,28,33	0
3	PBZ	B	702	10/10	0.86	0.17	40,47,50,53	0
3	PBZ	E	705	10/10	0.87	0.14	14,30,31,32	0
3	PBZ	P	716	10/10	0.87	0.11	25,33,34,36	0
3	PBZ	O	715	10/10	0.88	0.15	37,39,46,48	0
3	PBZ	I	709	10/10	0.88	0.15	45,46,48,50	0
3	PBZ	J	710	10/10	0.89	0.14	38,39,42,42	0
3	PBZ	A	701	10/10	0.89	0.13	14,19,26,33	0
3	PBZ	K	711	10/10	0.90	0.12	32,36,39,42	0
3	PBZ	F	706	10/10	0.90	0.12	22,26,28,28	0
3	PBZ	D	704	10/10	0.92	0.11	17,21,22,24	0
2	CO	I	3	1/1	0.95	0.06	63,63,63,63	0
2	CO	E	2	1/1	0.98	0.07	35,35,35,35	0
2	CO	M	4	1/1	0.99	0.06	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.