



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2024 – 12:14 PM EDT

PDB ID : 2BDH
Title : Human Kallikrein 4 complex with zinc 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.1

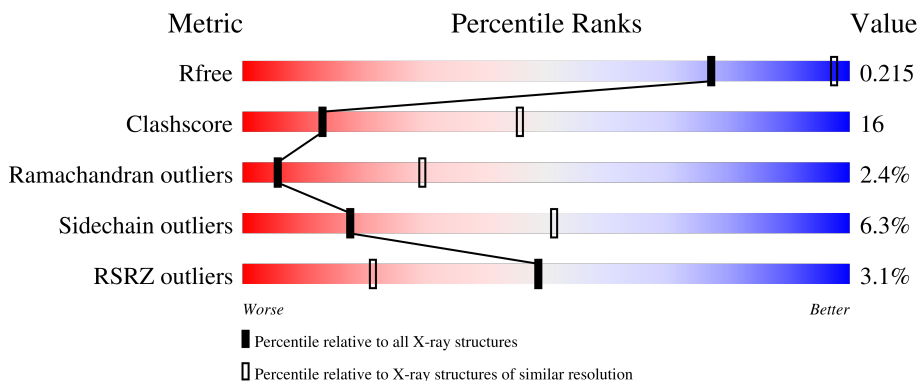
1 Overall quality at a glance i

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6832 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.

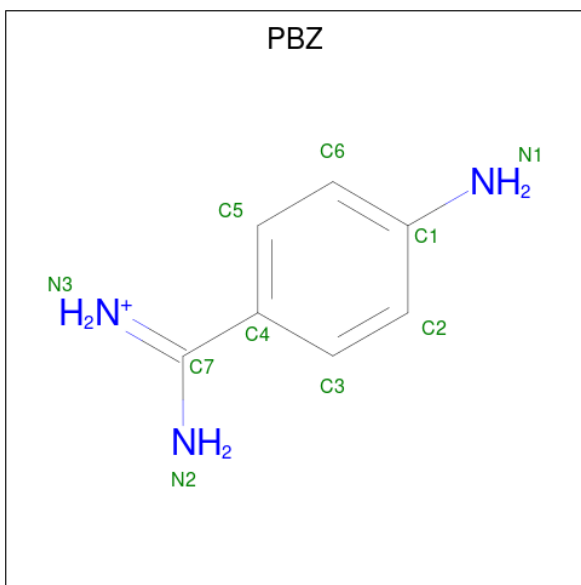
- Molecule 1 is a protein called Kallikrein-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	223	Total 1670	C 1043	N 281	O 329	S 17	55	0	0
1	B	223	Total 1670	C 1043	N 281	O 329	S 17	43	0	0
1	C	223	Total 1670	C 1043	N 281	O 329	S 17	35	0	0
1	D	223	Total 1670	C 1043	N 281	O 329	S 17	41	0	0

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

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

- Molecule 3 is P-AMINO BENZAMIDINE (three-letter code: 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

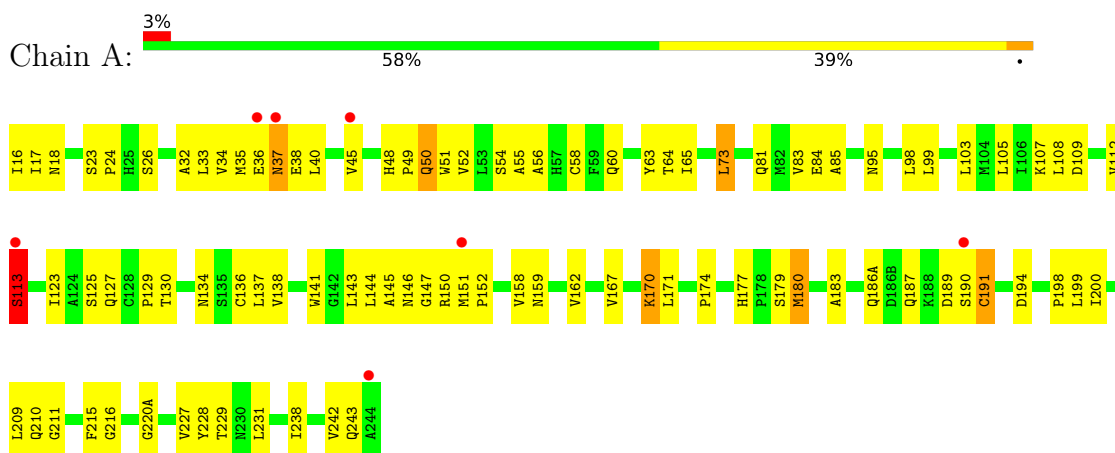
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	35	Total O 35 35	0	0
4	B	28	Total O 28 28	0	0
4	C	18	Total O 18 18	0	0
4	D	30	Total O 30 30	0	0

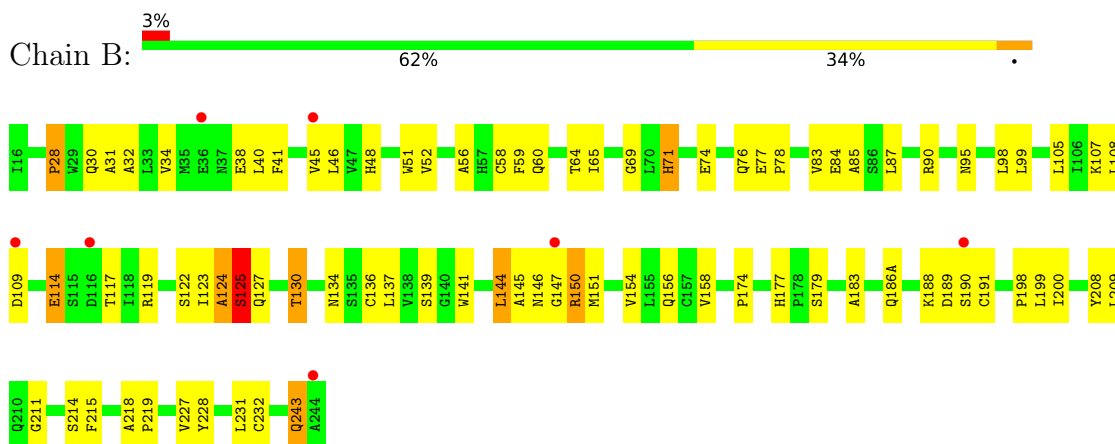
3 Residue-property plots [i](#)

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 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.

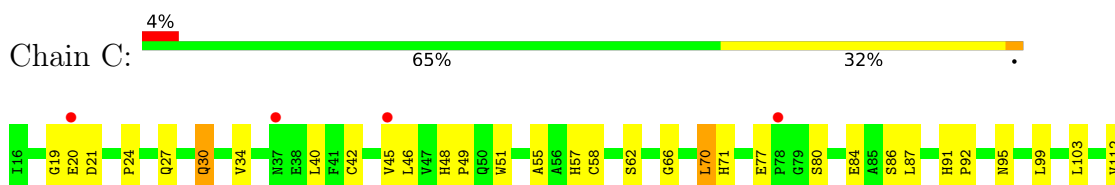
- Molecule 1: Kallikrein-4

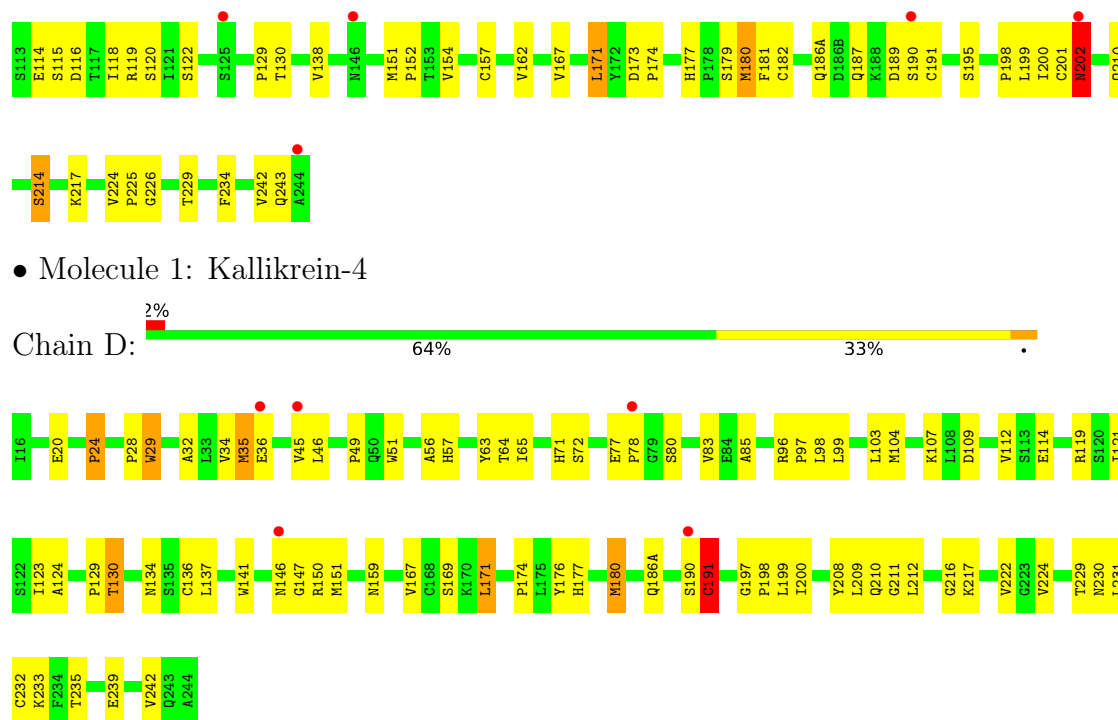


- Molecule 1: Kallikrein-4



- Molecule 1: Kallikrein-4





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	73.49Å 73.49Å 338.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.85 – 3.00 19.84 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.0 (19.85-3.00) 95.0 (19.84-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.71 (at 2.98Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.233 , 0.292 0.220 , 0.215	Depositor DCC
R_{free} test set	955 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	68.7	Xtrriage
Anisotropy	0.079	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6832	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.50	0/1707	0.70	1/2323 (0.0%)
1	B	0.45	0/1707	0.70	5/2323 (0.2%)
1	C	0.44	0/1707	0.62	0/2323
1	D	0.45	0/1707	0.66	2/2323 (0.1%)
All	All	0.46	0/6828	0.67	8/9292 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	SER	N-CA-C	6.98	129.84	111.00
1	D	151	MET	N-CA-C	-6.82	92.59	111.00
1	D	150	ARG	N-CA-C	6.70	129.08	111.00
1	B	127	GLN	N-CA-CB	-6.50	98.91	110.60
1	B	125	SER	N-CA-C	-5.73	95.53	111.00
1	B	151	MET	N-CA-C	-5.33	96.61	111.00
1	B	150	ARG	N-CA-C	5.14	124.87	111.00
1	B	125	SER	C-N-CA	5.08	134.41	121.70

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	A	1670	0	1598	57	0
1	B	1670	0	1598	55	0
1	C	1670	0	1598	52	0
1	D	1670	0	1598	48	0
2	A	1	0	0	0	0
3	A	10	0	10	2	0
3	B	10	0	10	0	0
3	C	10	0	10	0	0
3	D	10	0	10	3	0
4	A	35	0	0	2	0
4	B	28	0	0	2	0
4	C	18	0	0	0	0
4	D	30	0	0	1	0
All	All	6832	0	6432	208	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 16.

All (208) 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:D:77:GLU:HB2	1:D:80:SER:HB3	1.27	1.14
1:A:18:ASN:H	1:A:145:ALA:HB2	1.38	0.89
1:D:216:GLY:HA3	3:D:304:PBZ:HN22	1.47	0.79
1:B:45:VAL:HG11	1:B:209:LEU:HD22	1.66	0.75
1:D:28:PRO:HB2	1:D:119:ARG:H	1.51	0.75
1:D:186(A):GLN:HE21	1:D:222:VAL:HG11	1.51	0.74
1:B:48:HIS:HB3	1:B:51:TRP:HB2	1.71	0.73
1:C:115:SER:HB3	1:C:118:ILE:HB	1.70	0.73
1:A:48:HIS:HB3	1:A:51:TRP:HB2	1.71	0.73
1:C:95:ASN:HD22	1:C:99:LEU:H	1.36	0.71
1:A:17:ILE:HD11	1:A:191:CYS:HB2	1.73	0.70
1:C:186(A):GLN:HG2	1:D:57:HIS:CG	2.28	0.69
1:B:144:LEU:HB2	1:B:150:ARG:O	1.93	0.68
1:A:17:ILE:HG23	1:A:145:ALA:HA	1.74	0.68
1:B:45:VAL:HG22	1:B:198:PRO:HB3	1.75	0.67
1:C:186(A):GLN:HG2	1:D:57:HIS:CD2	2.30	0.67
1:A:170:LYS:HB2	1:B:174:PRO:HG3	1.77	0.66
1:C:95:ASN:ND2	1:C:99:LEU:H	1.94	0.66
1:C:45:VAL:CG2	1:C:198:PRO:HB3	2.26	0.65
1:A:123:ILE:HD12	1:A:123:ILE:H	1.61	0.65
1:A:211:GLY:HA2	1:A:231:LEU:HG	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:VAL:HG12	1:B:40:LEU:HA	1.79	0.63
1:A:73:LEU:HD12	1:A:73:LEU:H	1.62	0.63
1:D:167:VAL:O	1:D:171:LEU:HB2	1.98	0.62
1:C:151:MET:SD	1:C:152:PRO:HD2	2.39	0.62
1:C:66:GLY:HA3	1:C:70:LEU:HD11	1.83	0.61
1:B:137:LEU:HD12	1:B:158:VAL:O	2.02	0.60
1:C:167:VAL:O	1:C:171:LEU:HB2	2.02	0.60
1:A:177:HIS:HD2	1:A:179:SER:OG	1.85	0.59
1:A:32:ALA:HB2	1:A:141:TRP:CZ3	2.36	0.59
1:B:59:PHE:HB2	1:B:90:ARG:HD3	1.84	0.59
1:C:177:HIS:O	1:C:180:MET:HG3	2.02	0.59
1:A:190:SER:HB2	3:A:303:PBZ:HN32	1.67	0.58
1:C:45:VAL:HG22	1:C:198:PRO:HB3	1.86	0.58
1:A:144:LEU:HD21	1:A:152:PRO:HB3	1.84	0.57
1:D:34:VAL:HG22	1:D:64:THR:O	2.04	0.57
1:B:114:GLU:HG2	1:B:119:ARG:HA	1.87	0.57
1:A:187:GLN:HG2	1:A:220(A):GLY:O	2.05	0.57
1:B:200:ILE:HA	1:B:208:TYR:O	2.05	0.57
1:A:52:VAL:HG21	1:A:65:ILE:HD13	1.88	0.56
1:D:45:VAL:HG22	1:D:198:PRO:HB3	1.88	0.56
1:B:85:ALA:HB2	1:B:108:LEU:HA	1.88	0.56
1:B:218:ALA:HA	1:B:219:PRO:C	2.27	0.56
1:D:186(A):GLN:HE21	1:D:222:VAL:CG1	2.17	0.56
1:C:119:ARG:NH1	1:C:119:ARG:HB2	2.20	0.55
1:D:28:PRO:HB2	1:D:119:ARG:N	2.20	0.55
1:C:34:VAL:HG12	1:C:40:LEU:HA	1.87	0.55
1:C:177:HIS:HD2	1:C:179:SER:H	1.53	0.55
1:A:83:VAL:HG21	1:A:108:LEU:HD22	1.89	0.55
1:D:29:TRP:CE3	1:D:121:ILE:HB	2.41	0.55
1:C:48:HIS:HB3	1:C:51:TRP:HB2	1.88	0.54
1:A:49:PRO:O	1:A:112:VAL:HG22	2.07	0.54
1:B:158:VAL:HG22	1:B:188:LYS:HD3	1.89	0.54
1:B:177:HIS:CD2	1:B:179:SER:H	2.26	0.53
1:D:51:TRP:CZ3	1:D:107:LYS:HB2	2.44	0.53
1:B:189:ASP:CG	1:B:190:SER:H	2.12	0.53
1:D:186(A):GLN:NE2	1:D:222:VAL:HG11	2.21	0.53
1:A:199:LEU:HD12	1:A:228:TYR:CE2	2.44	0.53
1:A:45:VAL:HG22	1:A:198:PRO:HB3	1.89	0.52
1:D:35:MET:HB3	1:D:36:GLU:OE2	2.09	0.52
1:D:51:TRP:CD1	1:D:242:VAL:HG13	2.45	0.52
1:A:136:CYS:HB3	1:A:200:ILE:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:VAL:CG2	1:A:198:PRO:HB3	2.40	0.52
1:A:190:SER:HB2	3:A:303:PBZ:N3	2.26	0.51
1:B:32:ALA:HB2	1:B:141:TRP:CZ3	2.45	0.51
1:C:179:SER:HB2	1:C:234:PHE:HZ	1.76	0.51
1:C:20:GLU:O	1:C:157:CYS:N	2.37	0.51
1:C:45:VAL:HG21	1:C:198:PRO:HB3	1.92	0.50
1:A:189:ASP:CG	1:A:190:SER:H	2.14	0.50
1:B:199:LEU:HD12	1:B:228:TYR:CE2	2.46	0.50
1:D:45:VAL:HG11	1:D:209:LEU:HD22	1.93	0.50
1:D:217:LYS:HB2	1:D:224:VAL:HG11	1.94	0.50
1:A:81:GLN:NE2	1:A:113:SER:OG	2.45	0.50
1:B:144:LEU:HD23	1:B:145:ALA:H	1.75	0.50
1:C:49:PRO:O	1:C:112:VAL:HG22	2.12	0.50
1:D:32:ALA:HB2	1:D:141:TRP:CZ3	2.46	0.50
1:B:139:SER:HA	1:B:156:GLN:O	2.12	0.50
1:A:98:LEU:O	1:A:99:LEU:HB2	2.12	0.49
1:A:199:LEU:HD12	1:A:228:TYR:CD2	2.47	0.49
1:B:83:VAL:HG12	1:B:84:GLU:N	2.28	0.49
1:D:199:LEU:CD2	1:D:210:GLN:HB3	2.43	0.49
1:B:215:PHE:CE1	1:B:227:VAL:HG21	2.47	0.49
1:C:71:HIS:CE1	1:C:154:VAL:HB	2.48	0.49
1:C:77:GLU:O	1:C:80:SER:HB3	2.13	0.49
1:D:129:PRO:HG3	1:D:210:GLN:CG	2.43	0.49
1:D:137:LEU:HD12	1:D:159:ASN:HD21	1.78	0.48
1:B:40:LEU:HD13	1:B:41:PHE:N	2.28	0.48
1:A:134:ASN:O	1:A:162:VAL:HG23	2.14	0.48
1:B:130:THR:O	1:B:134:ASN:HB2	2.13	0.48
1:A:183:ALA:HB3	1:A:228:TYR:CE1	2.48	0.48
1:C:189:ASP:CG	1:C:190:SER:H	2.17	0.48
1:A:95:ASN:ND2	1:A:99:LEU:H	2.10	0.48
1:B:136:CYS:HB3	1:B:200:ILE:O	2.13	0.48
1:A:123:ILE:HD12	1:A:123:ILE:N	2.28	0.47
1:C:201:CYS:O	1:C:202:ASN:C	2.52	0.47
1:D:46:LEU:HD12	1:D:51:TRP:O	2.14	0.47
1:D:96:ARG:N	1:D:97:PRO:O	2.46	0.47
1:C:55:ALA:O	1:C:58:CYS:HB2	2.14	0.47
1:D:45:VAL:CG2	1:D:198:PRO:HB3	2.43	0.47
1:A:189:ASP:CG	1:A:190:SER:N	2.68	0.47
1:C:19:GLY:HA3	1:C:157:CYS:O	2.15	0.47
1:A:137:LEU:HD12	1:A:159:ASN:OD1	2.14	0.47
1:B:123:ILE:HG22	1:B:124:ALA:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:LYS:HB2	1:C:224:VAL:HG11	1.97	0.46
1:A:143:LEU:HA	1:A:150:ARG:O	2.16	0.46
1:A:54:SER:OG	1:A:55:ALA:N	2.48	0.46
1:B:34:VAL:HG22	1:B:64:THR:O	2.16	0.46
1:C:173:ASP:OD2	1:C:174:PRO:HA	2.16	0.46
1:A:85:ALA:HB1	1:A:107:LYS:O	2.16	0.46
1:A:138:VAL:HG13	1:A:158:VAL:HG12	1.97	0.46
1:B:76:GLN:OE1	1:B:76:GLN:HA	2.16	0.46
1:B:232:CYS:HB2	4:B:308:HOH:O	2.16	0.46
1:C:138:VAL:HG23	1:C:198:PRO:O	2.16	0.45
1:D:191:CYS:HA	3:D:304:PBZ:HN32	1.81	0.45
1:B:189:ASP:HB2	4:B:314:HOH:O	2.17	0.45
1:A:51:TRP:NE1	1:A:242:VAL:HG13	2.32	0.45
4:A:405:HOH:O	1:D:186(A):GLN:HG3	2.15	0.45
1:B:177:HIS:HD2	1:B:179:SER:H	1.62	0.45
1:D:136:CYS:HB3	1:D:200:ILE:O	2.16	0.45
1:A:103:LEU:HB3	1:A:229:THR:HG21	1.99	0.45
1:D:98:LEU:O	1:D:99:LEU:HB2	2.16	0.45
1:C:177:HIS:CD2	1:C:179:SER:H	2.32	0.45
1:B:30:GLN:HG3	1:B:31:ALA:N	2.31	0.45
1:B:40:LEU:HD13	1:B:40:LEU:C	2.37	0.45
1:B:56:ALA:C	1:B:58:CYS:H	2.19	0.45
1:B:87:LEU:HB3	1:B:107:LYS:HB3	1.98	0.45
1:A:33:LEU:O	1:A:40:LEU:HD22	2.17	0.45
1:A:167:VAL:HG12	1:A:171:LEU:HD12	1.97	0.45
1:C:46:LEU:HD12	1:C:51:TRP:O	2.17	0.45
1:C:181:PHE:HZ	1:C:199:LEU:HD23	1.82	0.45
1:A:84:GLU:O	1:A:109:ASP:HB2	2.17	0.44
1:C:30:GLN:HE21	1:C:30:GLN:HB2	1.65	0.44
1:C:129:PRO:HG3	1:C:210:GLN:CG	2.47	0.44
1:C:200:ILE:HG22	1:C:202:ASN:N	2.32	0.44
1:B:189:ASP:CG	1:B:190:SER:N	2.70	0.44
1:C:51:TRP:CD1	1:C:242:VAL:HG13	2.52	0.44
1:D:177:HIS:O	1:D:180:MET:HG3	2.17	0.44
1:A:56:ALA:C	1:A:58:CYS:H	2.21	0.44
1:A:215:PHE:CZ	1:A:227:VAL:HG21	2.52	0.44
1:B:211:GLY:HA2	1:B:231:LEU:HG	2.00	0.44
1:D:130:THR:O	1:D:134:ASN:HB2	2.18	0.44
1:C:129:PRO:HG3	1:C:210:GLN:CD	2.37	0.44
1:B:51:TRP:CZ3	1:B:105:LEU:HB3	2.52	0.44
1:D:78:PRO:HA	4:D:311:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:CYS:SG	1:D:233:LYS:HG2	2.58	0.44
1:B:95:ASN:ND2	1:B:99:LEU:H	2.15	0.44
1:D:211:GLY:HA2	1:D:231:LEU:HG	1.99	0.43
1:B:98:LEU:HG	1:B:99:LEU:HG	2.00	0.43
1:D:197:GLY:O	1:D:212:LEU:HA	2.18	0.43
1:A:37:ASN:OD1	1:A:37:ASN:N	2.50	0.43
1:A:60:GLN:HB2	1:A:63:TYR:CE2	2.53	0.43
1:A:194:ASP:HA	4:A:403:HOH:O	2.18	0.43
1:B:183:ALA:HB3	1:B:228:TYR:CE1	2.53	0.43
1:D:103:LEU:HB3	1:D:229:THR:HG21	2.00	0.43
1:D:85:ALA:HA	1:D:109:ASP:CG	2.38	0.43
1:B:28:PRO:HB2	1:B:119:ARG:N	2.33	0.43
1:B:71:HIS:CD2	1:B:154:VAL:HB	2.53	0.43
1:D:49:PRO:O	1:D:112:VAL:HG22	2.19	0.43
1:C:34:VAL:HG13	1:C:40:LEU:HD23	2.01	0.43
1:C:48:HIS:ND1	1:C:49:PRO:HD2	2.34	0.43
1:C:62:SER:HA	1:C:86:SER:HA	2.00	0.43
1:A:177:HIS:O	1:A:180:MET:HG3	2.18	0.43
1:B:45:VAL:CG2	1:B:198:PRO:HB3	2.44	0.42
1:B:46:LEU:HD12	1:B:51:TRP:O	2.19	0.42
1:D:65:ILE:O	1:D:83:VAL:HG22	2.18	0.42
1:B:59:PHE:CB	1:B:90:ARG:HD3	2.49	0.42
1:C:87:LEU:C	1:C:87:LEU:HD23	2.40	0.42
1:D:124:ALA:HB2	1:D:208:TYR:HB3	2.01	0.42
1:D:199:LEU:HD23	1:D:210:GLN:HB3	2.00	0.42
1:A:50:GLN:HE21	1:A:50:GLN:HB2	1.56	0.42
1:C:91:HIS:ND1	1:C:92:PRO:HD2	2.34	0.42
1:C:182:CYS:HB3	1:C:225:PRO:HB2	2.01	0.42
1:C:103:LEU:HB3	1:C:229:THR:HG21	2.01	0.42
1:A:16:ILE:N	1:A:194:ASP:OD2	2.53	0.41
1:A:45:VAL:HG11	1:A:209:LEU:HD22	2.01	0.41
1:B:69:GLY:HA2	1:B:117:THR:O	2.20	0.41
1:B:83:VAL:HG12	1:B:84:GLU:H	1.85	0.41
1:C:24:PRO:HG3	1:C:71:HIS:CD2	2.55	0.41
1:A:23:SER:HB2	1:A:26:SER:HB3	2.02	0.41
1:A:105:LEU:HD11	1:A:238:ILE:HG23	2.02	0.41
1:B:52:VAL:HG21	1:B:65:ILE:HD13	2.02	0.41
1:D:121:ILE:HD13	1:D:200:ILE:HD12	2.02	0.41
1:D:190:SER:C	3:D:304:PBZ:HN32	2.24	0.41
1:B:74:GLU:OE1	1:B:76:GLN:HB2	2.20	0.41
1:C:182:CYS:HA	1:C:226:GLY:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:SER:HA	1:D:176:TYR:CG	2.56	0.41
1:C:130:THR:O	1:C:162:VAL:HB	2.21	0.41
1:C:40:LEU:HD21	1:C:42:CYS:O	2.20	0.41
1:C:70:LEU:HD23	1:C:70:LEU:N	2.36	0.41
1:C:57:HIS:CE1	1:C:195:SER:HB3	2.56	0.41
1:A:34:VAL:HG23	1:A:64:THR:HB	2.03	0.41
1:B:58:CYS:O	1:B:60:GLN:HG2	2.21	0.41
1:B:99:LEU:HB3	1:B:215:PHE:CE2	2.56	0.41
1:B:177:HIS:HD2	1:B:179:SER:OG	2.04	0.41
1:C:115:SER:OG	1:C:116:ASP:N	2.54	0.41
1:D:56:ALA:HA	1:D:104:MET:HB3	2.03	0.41
1:D:235:THR:O	1:D:239:GLU:HB2	2.20	0.41
1:A:17:ILE:CG2	1:A:145:ALA:HA	2.47	0.41
1:A:129:PRO:HG3	1:A:210:GLN:CG	2.50	0.41
1:A:151:MET:HA	1:A:152:PRO:HD2	1.90	0.40
1:B:77:GLU:OE2	1:B:77:GLU:HA	2.20	0.40
1:B:84:GLU:O	1:B:109:ASP:HB2	2.21	0.40
1:B:186(A):GLN:NE2	1:C:214:SER:O	2.53	0.40
1:C:181:PHE:CZ	1:C:199:LEU:HD23	2.57	0.40
1:A:215:PHE:CD1	1:A:216:GLY:N	2.89	0.40
1:D:137:LEU:HD12	1:D:159:ASN:ND2	2.36	0.40
1:A:130:THR:O	1:A:134:ASN:HB2	2.22	0.40
1:D:123:ILE:HG22	1:D:124:ALA:N	2.35	0.40

There are no symmetry-related clashes.

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%)	199 (90%)	19 (9%)	3 (1%)	11 43
1	B	221/223 (99%)	184 (83%)	28 (13%)	9 (4%)	3 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	221/223 (99%)	191 (86%)	26 (12%)	4 (2%)	8	37
1	D	221/223 (99%)	186 (84%)	30 (14%)	5 (2%)	6	30
All	All	884/892 (99%)	760 (86%)	103 (12%)	21 (2%)	6	29

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	GLU
1	B	124	ALA
1	C	114	GLU
1	D	191	CYS
1	B	71	HIS
1	C	187	GLN
1	C	202	ASN
1	D	71	HIS
1	D	114	GLU
1	B	243	GLN
1	D	147	GLY
1	A	24	PRO
1	B	78	PRO
1	B	114	GLU
1	B	125	SER
1	B	146	ASN
1	C	243	GLN
1	D	24	PRO
1	A	147	GLY
1	B	147	GLY
1	B	28	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%)	174 (92%)	15 (8%)	12	41
1	B	189/189 (100%)	181 (96%)	8 (4%)	30	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	189/189 (100%)	177 (94%)	12 (6%)	18	51
1	D	189/189 (100%)	176 (93%)	13 (7%)	15	48
All	All	756/756 (100%)	708 (94%)	48 (6%)	18	51

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	MET
1	A	37	ASN
1	A	38	GLU
1	A	50	GLN
1	A	73	LEU
1	A	113	SER
1	A	125	SER
1	A	127	GLN
1	A	146	ASN
1	A	170	LYS
1	A	174	PRO
1	A	180	MET
1	A	186(A)	GLN
1	A	191	CYS
1	A	243	GLN
1	B	38	GLU
1	B	122	SER
1	B	125	SER
1	B	130	THR
1	B	144	LEU
1	B	191	CYS
1	B	214	SER
1	B	243	GLN
1	C	21	ASP
1	C	27	GLN
1	C	30	GLN
1	C	70	LEU
1	C	84	GLU
1	C	120	SER
1	C	122	SER
1	C	171	LEU
1	C	180	MET
1	C	191	CYS
1	C	202	ASN

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Mol	Chain	Res	Type
1	C	214	SER
1	D	20	GLU
1	D	24	PRO
1	D	29	TRP
1	D	35	MET
1	D	63	TYR
1	D	72	SER
1	D	130	THR
1	D	146	ASN
1	D	171	LEU
1	D	174	PRO
1	D	180	MET
1	D	191	CYS
1	D	230	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	50	GLN
1	A	60	GLN
1	A	95	ASN
1	A	177	HIS
1	A	186(A)	GLN
1	A	202	ASN
1	A	221	GLN
1	B	18	ASN
1	B	30	GLN
1	B	50	GLN
1	B	95	ASN
1	B	101	ASN
1	B	177	HIS
1	B	202	ASN
1	C	18	ASN
1	C	30	GLN
1	C	50	GLN
1	C	71	HIS
1	C	95	ASN
1	C	101	ASN
1	C	127	GLN
1	C	177	HIS
1	C	186(A)	GLN

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Mol	Chain	Res	Type
1	D	30	GLN
1	D	50	GLN
1	D	60	GLN
1	D	76	GLN
1	D	95	ASN
1	D	101	ASN
1	D	159	ASN
1	D	177	HIS
1	D	186(A)	GLN
1	D	187	GLN
1	D	202	ASN
1	D	210	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is 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	PBZ	B	301	-	10,10,10	1.94	4 (40%)	9,13,13	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PBZ	C	302	-	10,10,10	2.11	6 (60%)	9,13,13	0.62	0
3	PBZ	D	304	-	10,10,10	1.88	4 (40%)	9,13,13	0.59	0
3	PBZ	A	303	-	10,10,10	1.88	4 (40%)	9,13,13	0.74	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PBZ	B	301	-	-	0/4/4/4	0/1/1/1
3	PBZ	C	302	-	-	0/4/4/4	0/1/1/1
3	PBZ	D	304	-	-	4/4/4/4	0/1/1/1
3	PBZ	A	303	-	-	0/4/4/4	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	303	PBZ	C4-C7	3.67	1.54	1.47
3	B	301	PBZ	C4-C7	3.26	1.53	1.47
3	B	301	PBZ	C5-C4	2.95	1.44	1.39
3	C	302	PBZ	C4-C7	2.94	1.52	1.47
3	C	302	PBZ	C5-C4	2.88	1.44	1.39
3	D	304	PBZ	C3-C2	2.83	1.43	1.38
3	C	302	PBZ	C3-C4	2.72	1.44	1.39
3	C	302	PBZ	C3-C2	2.60	1.43	1.38
3	D	304	PBZ	C6-C5	2.46	1.43	1.38
3	A	303	PBZ	C3-C4	2.37	1.43	1.39
3	B	301	PBZ	C6-C5	2.30	1.42	1.38
3	A	303	PBZ	C5-C4	2.29	1.43	1.39
3	D	304	PBZ	C3-C4	2.22	1.43	1.39
3	B	301	PBZ	C3-C4	2.17	1.43	1.39
3	C	302	PBZ	C2-C1	2.14	1.44	1.40
3	C	302	PBZ	C6-C5	2.07	1.42	1.38
3	A	303	PBZ	C6-C5	2.04	1.42	1.38
3	D	304	PBZ	C4-C7	2.01	1.51	1.47

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	304	PBZ	C3-C4-C7-N2
3	D	304	PBZ	C5-C4-C7-N2
3	D	304	PBZ	C3-C4-C7-N3
3	D	304	PBZ	C5-C4-C7-N3

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	304	PBZ	3	0
3	A	303	PBZ	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	223/223 (100%)	-0.20	7 (3%)	49	21	28, 49, 81, 95	18 (8%)
1	B	223/223 (100%)	-0.21	7 (3%)	49	21	27, 51, 76, 94	14 (6%)
1	C	223/223 (100%)	-0.03	9 (4%)	38	15	29, 57, 86, 95	15 (6%)
1	D	223/223 (100%)	-0.06	5 (2%)	62	33	28, 57, 87, 97	14 (6%)
All	All	892/892 (100%)	-0.13	28 (3%)	49	21	27, 54, 84, 97	61 (6%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	45	VAL	3.9
1	B	116	ASP	3.7
1	B	244	ALA	3.5
1	A	45	VAL	3.5
1	C	190	SER	3.3
1	A	37	ASN	3.3
1	C	244	ALA	3.2
1	A	244	ALA	3.2
1	B	45	VAL	3.0
1	D	36	GLU	2.9
1	B	36	GLU	2.9
1	D	190	SER	2.9
1	C	45	VAL	2.7
1	C	146	ASN	2.5
1	C	125	SER	2.5
1	C	202	ASN	2.5
1	D	146	ASN	2.5
1	B	147	GLY	2.4
1	B	190	SER	2.3
1	C	37	ASN	2.3
1	A	151	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	109	ASP	2.2
1	C	78	PRO	2.2
1	A	190	SER	2.2
1	C	20	GLU	2.2
1	D	78	PRO	2.1
1	A	36	GLU	2.0
1	A	113	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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PBZ	C	302	10/10	0.86	0.26	55,57,58,59	0
3	PBZ	D	304	10/10	0.89	0.25	45,48,55,55	0
2	ZN	A	401	1/1	0.93	0.04	58,58,58,58	0
3	PBZ	B	301	10/10	0.93	0.21	44,48,51,52	0
3	PBZ	A	303	10/10	0.94	0.20	39,44,46,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.