



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:54 PM UTC

PDB ID : 6EBN / pdb_00006ebn
Title : Crystal structure of Psilocybe cubensis noncanonical aromatic amino acid de-carboxylase
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Deposited on : 2018-08-06
Resolution : 1.97 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	:	4-5-2 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

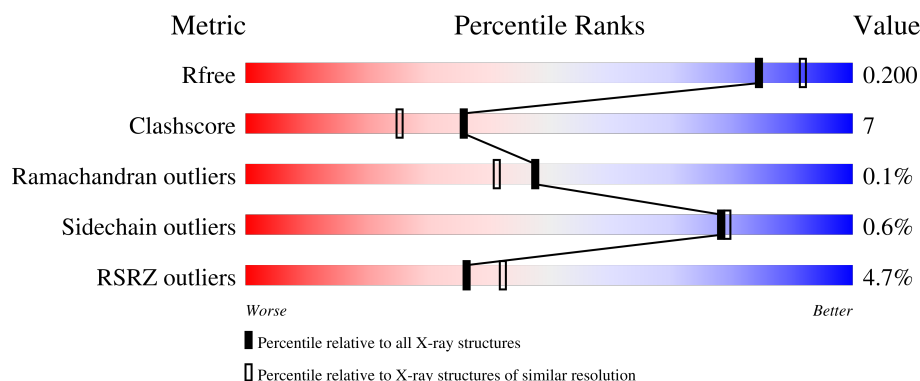
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	1013	4% 83% 12% • 5%
1	B	1013	5% 82% 12% • 5%

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	FMT	A	1107	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 16366 atoms, of which 64 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 non canonical aromatic amino acid decarboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	961	Total	C	N	O	P	S	0	13	0
			7680	4863	1310	1474	1	32			
1	B	958	Total	C	N	O	P	S	0	5	0
			7581	4802	1288	1458	1	32			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			5	1	2	2		
3	A	1	Total	C	H	O	0	0
			5	1	2	2		
3	A	1	Total	C	H	O	0	0
			5	1	2	2		
3	A	1	Total	C	H	O	0	0
			5	1	2	2		
3	A	1	Total	C	H	O	0	0
			5	1	2	2		
3	B	1	Total	C	H	O	0	0
			5	1	2	2		
3	B	1	Total	C	H	O	0	0
			5	1	2	2		
3	B	1	Total	C	H	O	0	0
			5	1	2	2		
3	B	1	Total	C	H	O	0	0
			5	1	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			5	1	2	2		
3	B	1	Total	C	H	O	0	0
			5	1	2	2		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Na	0	0
			2	2		
4	B	2	Total	Na	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	503	Total	O	0	0
			503	503		
5	B	468	Total	O	0	0
			468	468		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	238.72Å 143.57Å 71.41Å 90.00° 92.78° 90.00°	Depositor
Resolution (Å)	71.78 – 1.97 71.78 – 1.97	Depositor EDS
% Data completeness (in resolution range)	89.7 (71.78-1.97) 89.5 (71.78-1.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.83 (at 1.97Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.170 , 0.197 0.176 , 0.200	Depositor DCC
R_{free} test set	2001 reflections (1.19%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16366	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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: LLP, NA, FMT, GOL

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	0/7829	0.59	2/10642 (0.0%)
1	B	0.48	1/7727 (0.0%)	0.59	3/10505 (0.0%)
All	All	0.49	1/15556 (0.0%)	0.59	5/21147 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	47	ALA	C-O	-5.16	1.18	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	952	VAL	CB-CA-C	-6.89	105.85	111.71
1	B	353[A]	GLU	N-CA-C	5.62	119.86	112.89
1	B	353[B]	GLU	N-CA-C	5.62	119.86	112.89
1	A	353[A]	GLU	N-CA-C	5.35	118.27	111.69
1	A	353[B]	GLU	N-CA-C	5.35	118.27	111.69

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	7680	0	7516	108	0
1	B	7581	0	7422	120	0
2	A	18	24	23	3	0
2	B	12	16	15	5	0
3	A	18	12	6	3	0
3	B	18	12	6	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	503	0	0	4	0
5	B	468	0	0	13	0
All	All	16302	64	14988	220	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 7.

All (220) 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:A:724:THR:HG23	1:A:775:ILE:HD13	1.53	0.90
1:B:797:LEU:HD13	1:B:808:VAL:HG21	1.53	0.89
1:A:797:LEU:HD13	1:A:808:VAL:HG11	1.55	0.89
1:A:48:GLN:HE22	1:B:86:THR:HG23	1.36	0.86
1:A:315:VAL:HB	1:A:323:MET:HE2	1.58	0.84
1:A:799:ILE:O	1:A:802:ARG:HG2	1.79	0.82
1:B:799:ILE:CG2	1:B:802:ARG:HD2	2.09	0.81
1:A:724:THR:HG23	1:A:775:ILE:CD1	2.15	0.75
1:B:256:PRO:O	1:B:260:GLU:HG2	1.86	0.75
1:A:400:ARG:HD3	1:A:402:ARG:H	1.52	0.75
1:B:400:ARG:HD3	1:B:402:ARG:H	1.51	0.75
1:B:400:ARG:NH1	1:B:402:ARG:HG3	2.03	0.74
1:A:754:SER:OG	1:A:814:LYS:HB2	1.89	0.73
1:A:483:ILE:O	1:A:483:ILE:HG13	1.88	0.73
1:A:48:GLN:NE2	1:B:86:THR:HG23	2.04	0.72
1:B:483:ILE:O	1:B:483:ILE:HG13	1.89	0.72
1:B:400:ARG:HH11	1:B:401:ASN:H	1.36	0.72
1:B:761:VAL:O	1:B:762:ARG:NH1	2.24	0.71
1:A:457:ARG:HH12	3:A:1107:FMT:H	1.54	0.71
1:B:799:ILE:HG22	1:B:802:ARG:HD2	1.72	0.71
1:A:315:VAL:CB	1:A:323:MET:HE2	2.22	0.69
1:A:499:PHE:O	1:A:503[A]:GLU:HG2	1.92	0.68
1:A:789:ASP:OD1	1:A:815:VAL:HG22	1.94	0.67
1:A:864:ILE:HA	1:A:952:VAL:HG23	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:934:PRO:HB2	2:A:1103:GOL:H31	1.76	0.67
1:B:144:GLU:HG2	1:B:481:ILE:HD12	1.76	0.67
1:A:400:ARG:HH11	1:A:401:ASN:H	1.41	0.67
1:A:463:TYR:CD1	1:A:470:PRO:HG3	2.30	0.66
1:B:409:ASP:OD1	1:B:411:THR:HG23	1.95	0.65
1:A:144:GLU:CG	1:A:481:ILE:HD12	2.26	0.65
1:A:409:ASP:OD2	1:A:411:THR:HG23	1.97	0.64
1:B:929:THR:O	1:B:930:MET:HE2	1.98	0.64
1:B:315:VAL:HB	1:B:323:MET:HE2	1.79	0.63
1:B:761:VAL:HG11	1:B:797:LEU:HD22	1.81	0.63
1:B:222:LYS:HE2	3:B:1104:FMT:O1	1.98	0.63
1:B:872:VAL:HG21	1:B:881:LEU:HD11	1.80	0.62
1:A:289:LEU:HD23	1:A:313:ARG:HB2	1.82	0.62
1:A:797:LEU:HD13	1:A:808:VAL:CG1	2.29	0.62
1:B:777[B]:HIS:ND1	1:B:778:ASN:O	2.33	0.61
1:B:938:ILE:HD12	1:B:941:GLN:HG3	1.82	0.61
1:A:276:LEU:C	1:A:276:LEU:HD23	2.25	0.61
1:B:108:MET:SD	1:B:443:LLP:HE3	2.41	0.61
1:A:286:PRO:HB2	1:A:343:TYR:CZ	2.37	0.60
1:B:797:LEU:HD13	1:B:808:VAL:CG2	2.30	0.60
1:A:108:MET:SD	1:A:443:LLP:HE3	2.42	0.60
1:B:257:GLN:O	1:B:260:GLU:HG3	2.02	0.59
1:B:798:THR:HA	5:B:1208:HOH:O	2.02	0.59
1:A:353[B]:GLU:HG2	1:A:650:THR:HG21	1.83	0.59
1:B:523:CYS:SG	1:B:598:ASN:HA	2.43	0.59
1:A:19:ASP:OD2	1:A:417:HIS:HE1	1.86	0.58
1:B:275:THR:HG21	5:B:1421:HOH:O	2.02	0.58
1:B:757:VAL:HG13	1:B:808:VAL:HG11	1.86	0.58
1:A:144:GLU:HG2	1:A:481:ILE:HD12	1.83	0.58
1:A:758:GLU:HB2	1:A:809:LYS:HB3	1.86	0.58
1:A:797:LEU:CD1	1:A:808:VAL:HG21	2.33	0.58
1:A:279:ARG:NH2	5:A:1207:HOH:O	2.37	0.58
1:A:724:THR:CG2	1:A:775:ILE:HD13	2.32	0.57
1:B:400:ARG:HD3	1:B:401:ASN:N	2.18	0.57
1:B:722:ILE:HG23	1:B:777[B]:HIS:HD1	1.69	0.57
1:B:144:GLU:CG	1:B:481:ILE:HD12	2.35	0.57
1:B:265:LYS:HD2	5:B:1229:HOH:O	2.04	0.57
1:A:400:ARG:NH1	1:A:402:ARG:HG3	2.19	0.56
1:A:76[B]:GLN:OE1	1:B:405:LEU:HD11	2.05	0.56
1:A:279:ARG:HG3	5:A:1253:HOH:O	2.06	0.56
1:A:753:LEU:CD2	1:A:815:VAL:HG12	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:ARG:HD2	2:B:1102:GOL:C1	2.36	0.56
1:A:400:ARG:HD3	1:A:401:ASN:N	2.21	0.56
1:B:286:PRO:HB2	1:B:343:TYR:CZ	2.41	0.56
1:B:276:LEU:C	1:B:276:LEU:HD23	2.31	0.56
1:B:463:TYR:CD1	1:B:470:PRO:HG3	2.40	0.55
1:A:744:MET:HE3	5:A:1475:HOH:O	2.06	0.55
1:B:525:ARG:HD2	5:B:1393:HOH:O	2.06	0.55
1:A:144:GLU:HG3	1:A:481:ILE:HD12	1.88	0.55
1:A:731:GLY:CA	1:A:762:ARG:HH12	2.20	0.55
1:B:291:PRO:HD3	1:B:323:MET:HE3	1.89	0.54
1:B:45:VAL:O	1:B:49:GLN:HG2	2.07	0.54
1:A:807[A]:LYS:HD2	1:A:808:VAL:N	2.24	0.53
1:A:691:ASN:HB2	2:B:1101:GOL:H31	1.90	0.53
1:B:421:ARG:HD2	2:B:1102:GOL:H12	1.91	0.53
1:A:827[A]:GLU:O	1:A:853:VAL:HG22	2.09	0.53
1:B:260:GLU:O	1:B:264:ARG:HG3	2.09	0.53
1:A:95:ARG:HH11	1:A:95:ARG:HG2	1.73	0.52
1:A:933:ILE:O	1:A:933:ILE:HG13	2.09	0.52
1:B:788:VAL:HG12	5:B:1243:HOH:O	2.08	0.52
1:A:315:VAL:CG2	1:A:323:MET:HE2	2.40	0.52
1:B:483:ILE:O	1:B:483:ILE:CG1	2.58	0.52
1:B:633:VAL:HG21	1:B:640:PRO:HB3	1.92	0.52
1:A:523:CYS:SG	1:A:598:ASN:HA	2.49	0.51
1:A:794:ASP:HB3	1:A:807[A]:LYS:HE2	1.93	0.51
1:A:775:ILE:HD12	1:A:776:VAL:N	2.25	0.51
1:B:757:VAL:HG13	1:B:808:VAL:CG1	2.40	0.51
1:A:833:LEU:HD13	1:A:886:GLU:HA	1.93	0.51
1:B:273:LYS:HE3	5:B:1382:HOH:O	2.11	0.51
1:B:724:THR:HG23	1:B:775:ILE:HG13	1.92	0.51
1:B:930:MET:HE2	1:B:930:MET:HA	1.93	0.51
1:A:114:LEU:N	1:A:115:PRO:HD2	2.26	0.51
1:A:776:VAL:HG22	1:A:797:LEU:CD1	2.40	0.51
1:B:23:ILE:C	1:B:23:ILE:HD12	2.35	0.51
1:B:688:THR:HG22	1:B:694:VAL:HG22	1.92	0.51
1:A:45:VAL:O	1:A:49:GLN:HG2	2.11	0.50
1:A:405:LEU:HD23	1:A:405:LEU:H	1.76	0.50
1:A:421:ARG:HA	2:A:1102:GOL:H11	1.92	0.50
1:B:457:ARG:HH22	3:B:1105:FMT:H	1.75	0.50
1:A:815:VAL:O	1:A:815:VAL:HG23	2.11	0.50
1:B:802:ARG:HG2	1:B:802:ARG:HH21	1.75	0.50
1:A:633:VAL:HG21	1:A:640:PRO:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:TRP:CD2	1:B:465:LEU:HD22	2.47	0.50
1:A:421:ARG:NE	2:A:1102:GOL:O1	2.23	0.50
1:A:258:PHE:CG	1:B:892:SER:HA	2.47	0.50
1:A:775:ILE:HD11	1:A:777[B]:HIS:CE1	2.47	0.50
1:A:442:HIS:HA	1:A:447:VAL:O	2.12	0.49
1:A:50:LYS:HE2	5:B:1435:HOH:O	2.11	0.49
1:A:788:VAL:HG12	1:A:789:ASP:N	2.28	0.49
1:B:291:PRO:CD	1:B:323:MET:HE3	2.43	0.49
1:B:758:GLU:HB2	1:B:809:LYS:HB3	1.94	0.49
1:B:562:GLU:OE1	5:B:1201:HOH:O	2.20	0.49
1:A:841[A]:THR:HG22	1:A:842:GLN:N	2.28	0.49
1:B:933:ILE:HG13	1:B:933:ILE:O	2.12	0.49
1:A:775:ILE:HD11	1:A:777[B]:HIS:NE2	2.28	0.48
1:B:170:HIS:HE1	1:B:181:GLU:OE1	1.96	0.48
1:B:421:ARG:HA	2:B:1102:GOL:H31	1.93	0.48
1:A:457:ARG:HH22	3:A:1107:FMT:C	2.26	0.48
1:A:574:PHE:HA	1:A:692:ASP:OD2	2.14	0.48
1:A:854:VAL:HA	1:A:855:PRO:C	2.38	0.48
1:B:777[B]:HIS:CE1	1:B:778:ASN:O	2.67	0.48
1:B:799:ILE:CB	1:B:802:ARG:HD2	2.44	0.48
1:B:779:THR:CG2	1:B:796:ILE:HG13	2.44	0.47
1:B:722:ILE:CG2	1:B:777[B]:HIS:HD1	2.27	0.47
1:A:260:GLU:CG	1:A:469:ALA:H	2.27	0.47
1:B:61:ASN:HB2	2:B:1101:GOL:H11	1.95	0.47
1:A:406:PRO:HB2	1:A:408:GLU:HG2	1.97	0.46
1:B:95:ARG:HG2	1:B:95:ARG:HH21	1.80	0.46
1:A:872:VAL:HG21	1:A:881:LEU:HD11	1.96	0.46
1:B:689:THR:HA	1:B:694:VAL:HG23	1.97	0.46
1:A:731:GLY:HA3	1:A:762:ARG:HH12	1.80	0.46
1:B:799:ILE:N	1:B:799:ILE:HD12	2.29	0.46
1:A:23:ILE:HD12	1:A:23:ILE:C	2.41	0.46
1:A:170:HIS:HE1	1:A:181:GLU:OE1	1.99	0.46
1:B:595:SER:HB2	1:B:599:ILE:O	2.16	0.46
1:B:724:THR:HG23	1:B:775:ILE:HD11	1.96	0.46
1:B:481:ILE:HG23	1:B:481:ILE:O	2.14	0.46
1:B:461:MET:HE2	5:B:1431:HOH:O	2.16	0.46
1:B:763:GLN:O	1:B:763:GLN:HG2	2.16	0.46
1:A:286:PRO:HB2	1:A:343:TYR:CE2	2.51	0.46
1:B:753:LEU:CD2	1:B:815:VAL:HG22	2.46	0.46
1:B:775:ILE:HD11	1:B:777[A]:HIS:CE1	2.51	0.46
1:B:802:ARG:HG2	1:B:802:ARG:NH2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:PRO:CD	1:A:323:MET:HE3	2.46	0.45
1:A:776:VAL:HG22	1:A:797:LEU:HD12	1.97	0.45
1:A:929:THR:O	1:A:930:MET:HE2	2.15	0.45
1:B:854:VAL:HA	1:B:855:PRO:C	2.41	0.45
1:A:540:PHE:HB3	1:A:709:VAL:HG21	1.98	0.45
1:B:168:TRP:CH2	1:B:170:HIS:HB3	2.51	0.45
1:B:724:THR:HG23	1:B:775:ILE:CG1	2.47	0.45
1:A:273:LYS:HE3	5:A:1354:HOH:O	2.16	0.45
1:A:357:VAL:HG11	1:A:427:GLN:HB2	1.98	0.45
1:B:114:LEU:N	1:B:115:PRO:HD2	2.31	0.45
1:B:792:SER:HB2	1:B:809:LYS:HE2	1.98	0.45
1:B:357:VAL:HG11	1:B:427:GLN:HB2	1.99	0.45
1:B:194:LEU:N	1:B:194:LEU:HD12	2.32	0.45
1:B:292:SER:HA	1:B:314:ASN:HB3	1.99	0.45
1:B:279:ARG:HG3	5:B:1354:HOH:O	2.17	0.44
1:A:892:SER:HA	1:B:258:PHE:CG	2.53	0.44
1:B:794:ASP:OD2	1:B:809:LYS:HD3	2.17	0.44
1:A:400:ARG:CD	1:A:402:ARG:H	2.26	0.44
1:B:269:GLN:HG2	5:B:1557:HOH:O	2.18	0.44
1:B:318:ASP:O	1:B:660:CYS:HB2	2.17	0.44
1:A:483:ILE:O	1:A:483:ILE:CG1	2.62	0.44
1:B:788:VAL:HG22	1:B:789:ASP:N	2.33	0.44
1:B:799:ILE:HB	1:B:802:ARG:HD2	1.98	0.44
1:B:777[B]:HIS:NE2	1:B:796:ILE:HD12	2.32	0.44
1:A:938:ILE:HD12	1:A:941:GLN:HG3	2.00	0.44
1:B:265:LYS:CD	5:B:1229:HOH:O	2.63	0.44
1:B:315:VAL:CB	1:B:323:MET:HE2	2.47	0.44
1:A:291:PRO:HD3	1:A:323:MET:HE3	2.00	0.44
1:B:481:ILE:O	1:B:481:ILE:HG12	2.18	0.44
1:B:724:THR:HG23	1:B:775:ILE:CD1	2.47	0.44
1:B:808:VAL:HG12	1:B:809:LYS:N	2.33	0.44
1:A:86:THR:HG23	1:B:48:GLN:HE22	1.83	0.43
1:A:260:GLU:HG2	1:A:469:ALA:N	2.34	0.43
1:B:291:PRO:HD3	1:B:323:MET:CE	2.49	0.43
1:B:395:LYS:HA	1:B:395:LYS:HD3	1.89	0.43
1:B:574:PHE:HA	1:B:692:ASP:OD2	2.18	0.43
1:B:406:PRO:HB2	1:B:408:GLU:HG2	2.00	0.43
1:A:450:PRO:HG3	1:B:450:PRO:HG3	2.00	0.43
1:A:788:VAL:HG12	1:A:789:ASP:H	1.84	0.43
1:B:775:ILE:HG22	1:B:798:THR:O	2.18	0.43
1:A:395:LYS:HA	1:A:395:LYS:HD3	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:SER:HB2	1:A:599:ILE:O	2.18	0.43
1:A:799:ILE:HD12	1:A:799:ILE:N	2.33	0.42
1:B:328:LEU:HD23	1:B:366:LEU:HD12	2.01	0.42
1:B:400:ARG:CD	1:B:402:ARG:H	2.25	0.42
1:B:405:LEU:H	1:B:405:LEU:HD23	1.84	0.42
1:B:15:PRO:HB2	1:B:414:PHE:CE1	2.54	0.42
1:B:738:HIS:CE1	1:B:740:PRO:HA	2.55	0.42
1:A:755:VAL:HG12	1:A:813:ILE:HG12	2.01	0.42
1:B:839:TYR:CE2	1:B:846:HIS:HB2	2.54	0.42
1:A:291:PRO:HD3	1:A:323:MET:CE	2.50	0.42
1:A:827[A]:GLU:OE1	1:A:936:HIS:HE1	2.03	0.42
1:A:260:GLU:HG2	1:A:468:SER:HA	2.02	0.41
1:A:724:THR:H	3:A:1104:FMT:H	1.85	0.41
1:A:753:LEU:HD23	1:A:815:VAL:HA	2.03	0.41
1:B:925:TYR:OH	1:B:934:PRO:HD2	2.20	0.41
1:A:654:GLN:HG3	1:A:673:ASP:O	2.21	0.41
1:A:657:TYR:O	1:A:658:GLY:C	2.63	0.41
1:B:753:LEU:HD23	1:B:815:VAL:HA	2.02	0.41
1:A:792:SER:HB2	1:A:810:ILE:O	2.20	0.41
1:A:168:TRP:CH2	1:A:170:HIS:HB3	2.54	0.41
1:B:657:TYR:O	1:B:658:GLY:C	2.63	0.41
1:B:290:SER:O	1:B:314:ASN:HA	2.21	0.41
1:B:400:ARG:CZ	1:B:402:ARG:HG3	2.48	0.41
1:A:291:PRO:N	1:A:323:MET:HE3	2.36	0.41
1:A:796:ILE:CG2	1:A:805:SER:HB2	2.51	0.41
1:B:39:GLN:CD	5:B:1216:HOH:O	2.64	0.41
1:B:608:ASP:OD1	1:B:608:ASP:C	2.64	0.41
1:B:818:LYS:C	1:B:819:ARG:HD2	2.45	0.41
1:B:688:THR:O	1:B:693:PHE:HB3	2.21	0.40
1:A:57:PHE:CZ	1:B:644:PRO:HB3	2.56	0.40
1:A:816:VAL:O	1:A:817:LYS:HD3	2.22	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	969/1013 (96%)	943 (97%)	25 (3%)	1 (0%)	48	41
1	B	958/1013 (95%)	932 (97%)	25 (3%)	1 (0%)	48	41
All	All	1927/2026 (95%)	1875 (97%)	50 (3%)	2 (0%)	48	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	658	GLY
1	A	658	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	839/871 (96%)	834 (99%)	5 (1%)	78	79
1	B	829/871 (95%)	824 (99%)	5 (1%)	78	79
All	All	1668/1742 (96%)	1658 (99%)	10 (1%)	78	79

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	HIS
1	A	272	ASN
1	A	313	ARG
1	A	775	ILE
1	A	801	LYS
1	B	170	HIS
1	B	461	MET
1	B	762	ARG
1	B	775	ILE
1	B	872	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	170	HIS
1	A	284	GLN
1	A	322	HIS
1	A	344	GLN
1	A	546	ASN
1	A	889	HIS
1	A	907	GLN
1	A	940	ASN
1	B	48	GLN
1	B	170	HIS
1	B	320	GLN
1	B	322	HIS
1	B	344	GLN
1	B	417	HIS
1	B	546	ASN
1	B	733	GLN
1	B	907	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	LLP	A	443	1	23,24,25	2.62	7 (30%)	25,32,34	1.64	6 (24%)
1	LLP	B	443	1	23,24,25	2.46	7 (30%)	25,32,34	1.47	5 (20%)

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
1	LLP	A	443	1	-	4/16/17/19	0/1/1/1
1	LLP	B	443	1	-	4/16/17/19	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	443	LLP	C4-C4'	7.15	1.61	1.46
1	B	443	LLP	C4-C4'	7.12	1.61	1.46
1	A	443	LLP	C4'-NZ	5.53	1.45	1.27
1	B	443	LLP	C4'-NZ	5.21	1.44	1.27
1	A	443	LLP	C6-N1	3.81	1.42	1.34
1	B	443	LLP	C2'-C2	3.68	1.56	1.50
1	A	443	LLP	C2'-C2	3.42	1.55	1.50
1	B	443	LLP	C4-C5	-3.30	1.37	1.42
1	A	443	LLP	C5'-C5	3.23	1.59	1.50
1	A	443	LLP	C4-C5	-3.14	1.37	1.42
1	B	443	LLP	C5'-C5	2.56	1.57	1.50
1	B	443	LLP	P-OP2	-2.42	1.45	1.54
1	A	443	LLP	P-OP2	-2.42	1.45	1.54
1	B	443	LLP	C6-N1	2.28	1.39	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	443	LLP	C4-C4'-NZ	-4.27	104.33	124.04
1	B	443	LLP	C4-C4'-NZ	-3.79	106.55	124.04
1	A	443	LLP	C3-C4-C5	2.83	120.55	118.28
1	B	443	LLP	C3-C4-C5	2.66	120.42	118.28
1	A	443	LLP	C5-C6-N1	-2.37	119.97	123.83
1	A	443	LLP	OP3-P-OP2	2.35	116.61	107.80
1	A	443	LLP	C3-C4-C4'	-2.32	116.21	120.40
1	B	443	LLP	OP4-P-OP1	2.23	112.47	106.44
1	B	443	LLP	C5-C6-N1	-2.17	120.30	123.83
1	B	443	LLP	O3-C3-C2	2.16	122.05	117.58
1	A	443	LLP	C2'-C2-N1	2.15	121.69	117.64

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	443	LLP	C3-C4-C4'-NZ
1	A	443	LLP	C4-C4'-NZ-CE
1	A	443	LLP	O-C-CA-CB
1	B	443	LLP	C3-C4-C4'-NZ
1	B	443	LLP	C4-C4'-NZ-CE
1	B	443	LLP	O-C-CA-CB
1	A	443	LLP	CG-CD-CE-NZ
1	B	443	LLP	CG-CD-CE-NZ

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	443	LLP	1	0
1	B	443	LLP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 4 are monoatomic - leaving 17 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	FMT	B	1105	-	2,2,2	0.71	0	1,1,1	0.46	0
2	GOL	A	1103	-	5,5,5	1.19	1 (20%)	5,5,5	0.83	0
3	FMT	A	1109	-	2,2,2	0.71	0	1,1,1	0.46	0
3	FMT	B	1108	-	2,2,2	0.72	0	1,1,1	0.49	0
3	FMT	B	1104	-	2,2,2	0.93	0	1,1,1	0.63	0
3	FMT	B	1107	-	2,2,2	0.66	0	1,1,1	0.40	0
2	GOL	A	1101	-	5,5,5	1.35	0	5,5,5	0.96	0
3	FMT	A	1107	-	2,2,2	0.63	0	1,1,1	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	1102	-	5,5,5	1.59	1 (20%)	5,5,5	1.22	0
2	GOL	B	1102	-	5,5,5	1.56	1 (20%)	5,5,5	0.89	0
3	FMT	A	1104	-	2,2,2	0.63	0	1,1,1	0.36	0
3	FMT	A	1105	-	2,2,2	0.84	0	1,1,1	0.62	0
3	FMT	A	1108	-	2,2,2	0.66	0	1,1,1	0.35	0
3	FMT	A	1106	-	2,2,2	1.04	0	1,1,1	0.58	0
3	FMT	B	1106	-	2,2,2	0.72	0	1,1,1	0.47	0
3	FMT	B	1103	-	2,2,2	0.63	0	1,1,1	0.39	0
2	GOL	B	1101	-	5,5,5	0.72	0	5,5,5	1.09	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
2	GOL	A	1103	-	-	0/4/4/4	-
2	GOL	A	1101	-	-	2/4/4/4	-
2	GOL	A	1102	-	-	0/4/4/4	-
2	GOL	B	1102	-	-	3/4/4/4	-
2	GOL	B	1101	-	-	0/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1102	GOL	O2-C2	-3.18	1.34	1.43
2	B	1102	GOL	O2-C2	-3.04	1.34	1.43
2	A	1103	GOL	O2-C2	-2.10	1.37	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1102	GOL	C1-C2-C3-O3
2	B	1102	GOL	O2-C2-C3-O3
2	A	1101	GOL	C1-C2-C3-O3
2	A	1101	GOL	O2-C2-C3-O3
2	B	1102	GOL	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1105	FMT	1	0
2	A	1103	GOL	1	0
3	B	1104	FMT	1	0
3	A	1107	FMT	2	0
2	A	1102	GOL	2	0
2	B	1102	GOL	3	0
3	A	1104	FMT	1	0
2	B	1101	GOL	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	960/1013 (94%)	0.08	45 (4%)	36 42	14, 40, 82, 132	13 (1%)
1	B	957/1013 (94%)	0.16	46 (4%)	35 41	21, 42, 84, 130	5 (0%)
All	All	1917/2026 (94%)	0.12	91 (4%)	36 42	14, 41, 84, 132	18 (0%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	841[A]	THR	6.9
1	A	764	ALA	6.2
1	B	473	ALA	5.6
1	B	14	VAL	5.3
1	A	405	LEU	5.1
1	B	405	LEU	4.8
1	B	764	ALA	4.6
1	B	296	TYR	4.4
1	A	483	ILE	4.4
1	B	775	ILE	4.2
1	B	469	ALA	4.2
1	B	471	TYR	4.1
1	B	411	THR	4.0
1	B	904	ILE	4.0
1	A	469	ALA	3.9
1	B	977	VAL	3.9
1	B	771	VAL	3.8
1	A	14	VAL	3.8
1	B	412	SER	3.7
1	A	771	VAL	3.4
1	A	761	VAL	3.3
1	A	804	THR	3.3
1	A	412	SER	3.3
1	B	483	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	872	VAL	3.2
1	A	411	THR	3.1
1	B	472	LEU	3.0
1	B	761	VAL	3.0
1	A	473	ALA	3.0
1	A	980	ALA	3.0
1	B	797	LEU	3.0
1	A	777[A]	HIS	2.9
1	A	472	LEU	2.9
1	B	467	TRP	2.9
1	B	481	ILE	2.9
1	B	799	ILE	2.9
1	A	399	GLY	2.9
1	B	413	GLY	2.8
1	B	798	THR	2.8
1	A	400	ARG	2.8
1	B	804	THR	2.8
1	B	780	VAL	2.8
1	A	807[A]	LYS	2.8
1	A	788	VAL	2.8
1	A	797	LEU	2.7
1	B	476	ASN	2.7
1	B	903	LYS	2.7
1	B	470	PRO	2.6
1	A	902	PHE	2.6
1	A	757	VAL	2.6
1	A	936	HIS	2.6
1	A	796	ILE	2.6
1	B	800	GLY	2.5
1	B	777[A]	HIS	2.5
1	A	468	SER	2.5
1	B	774	VAL	2.5
1	A	798	THR	2.5
1	B	404	ARG	2.4
1	A	800	GLY	2.4
1	B	976	HIS	2.4
1	A	470	PRO	2.4
1	A	467	TRP	2.4
1	B	466	THR	2.4
1	A	161	ASN	2.4
1	B	906	ASN	2.3
1	B	902	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	915	ILE	2.3
1	B	468	SER	2.3
1	B	875	GLU	2.3
1	A	401	ASN	2.3
1	A	917	ARG	2.2
1	A	471	TYR	2.2
1	A	806	PHE	2.2
1	A	490[A]	LYS	2.2
1	B	806	PHE	2.1
1	A	904	ILE	2.1
1	B	763	GLN	2.1
1	A	293	THR	2.1
1	A	815	VAL	2.1
1	A	482	GLY	2.1
1	B	776	VAL	2.1
1	A	799	ILE	2.1
1	A	160	ASN	2.1
1	B	596	ASP	2.1
1	A	404	ARG	2.1
1	A	762	ARG	2.1
1	A	903	LYS	2.0
1	B	796	ILE	2.0
1	B	779	THR	2.0
1	A	474	GLN	2.0
1	B	755	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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($\text{\AA}^2$)	Q<0.9
1	LLP	A	443	24/25	0.97	0.08	25,32,41,48	0
1	LLP	B	443	24/25	0.97	0.07	23,34,43,49	0

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($\text{\AA}^2$)	Q<0.9
3	FMT	A	1109	3/3	0.79	0.16	70,71,84,85	0
2	GOL	A	1103	6/6	0.80	0.12	65,78,81,84	0
3	FMT	B	1105	3/3	0.82	0.15	76,77,92,94	0
2	GOL	A	1102	6/6	0.83	0.16	66,79,89,99	0
3	FMT	B	1103	3/3	0.85	0.12	68,69,81,84	0
3	FMT	A	1105	3/3	0.85	0.15	56,58,67,70	0
3	FMT	B	1107	3/3	0.85	0.13	66,67,80,80	0
2	GOL	B	1101	6/6	0.86	0.11	55,66,69,73	0
3	FMT	A	1104	3/3	0.87	0.14	70,71,84,87	0
3	FMT	B	1108	3/3	0.87	0.09	75,75,91,93	0
3	FMT	A	1108	3/3	0.88	0.12	53,57,69,71	0
2	GOL	A	1101	6/6	0.88	0.13	53,63,67,71	0
2	GOL	B	1102	6/6	0.88	0.12	59,70,79,85	0
3	FMT	B	1104	3/3	0.90	0.13	50,52,60,63	0
3	FMT	B	1106	3/3	0.90	0.16	64,64,77,77	0
4	NA	B	1110	1/1	0.90	0.11	40,40,40,40	0
3	FMT	A	1107	3/3	0.92	0.10	69,70,83,85	0
3	FMT	A	1106	3/3	0.95	0.08	37,45,48,57	0
4	NA	B	1109	1/1	0.98	0.04	24,24,24,24	0
4	NA	A	1110	1/1	0.98	0.09	17,17,17,17	0
4	NA	A	1111	1/1	0.99	0.07	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.