



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:15 AM UTC

PDB ID : 7ZPF / pdb_00007zpf
Title : Three-dimensional structure of AIP56, a short-trip single chain AB toxin from *Photobacterium damsela* subsp. *piscicida*.
Authors : Lisboa, J.; Pereira, P.J.B.; dos Santos, N.M.S.
Deposited on : 2022-04-27
Resolution : 2.54 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

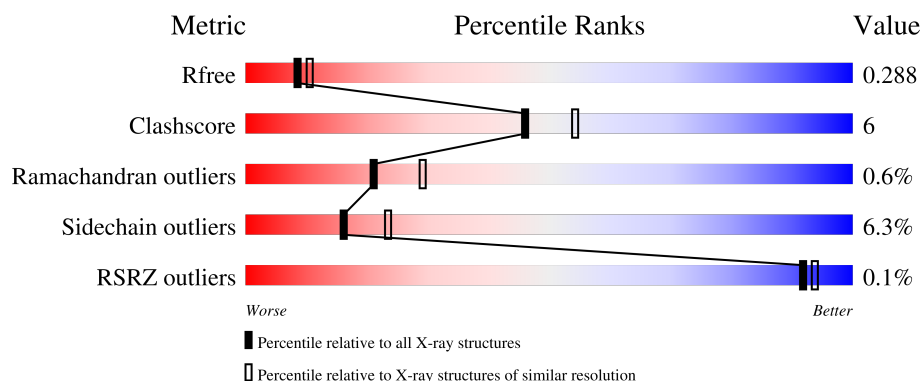
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	521	 73% 15% • 11%
1	B	521	 70% 16% • 13%
1	C	521	 69% 14% • 15%
1	D	521	 70% 15% • 14%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14880 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 Aip56.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3745	2380	644	715	6			
1	B	452	Total	C	N	O	S	0	0	0
			3662	2331	629	696	6			
1	C	445	Total	C	N	O	S	0	0	0
			3599	2291	621	681	6			
1	D	449	Total	C	N	O	S	0	0	0
			3629	2306	624	693	6			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	498	LEU	-	expression tag	UNP Q2VL32
A	499	GLU	-	expression tag	UNP Q2VL32
A	500	HIS	-	expression tag	UNP Q2VL32
A	501	HIS	-	expression tag	UNP Q2VL32
A	502	HIS	-	expression tag	UNP Q2VL32
A	503	HIS	-	expression tag	UNP Q2VL32
A	504	HIS	-	expression tag	UNP Q2VL32
A	505	HIS	-	expression tag	UNP Q2VL32
B	498	LEU	-	expression tag	UNP Q2VL32
B	499	GLU	-	expression tag	UNP Q2VL32
B	500	HIS	-	expression tag	UNP Q2VL32
B	501	HIS	-	expression tag	UNP Q2VL32
B	502	HIS	-	expression tag	UNP Q2VL32
B	503	HIS	-	expression tag	UNP Q2VL32
B	504	HIS	-	expression tag	UNP Q2VL32
B	505	HIS	-	expression tag	UNP Q2VL32
C	498	LEU	-	expression tag	UNP Q2VL32
C	499	GLU	-	expression tag	UNP Q2VL32
C	500	HIS	-	expression tag	UNP Q2VL32
C	501	HIS	-	expression tag	UNP Q2VL32
C	502	HIS	-	expression tag	UNP Q2VL32

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Chain	Residue	Modelled	Actual	Comment	Reference
C	503	HIS	-	expression tag	UNP Q2VL32
C	504	HIS	-	expression tag	UNP Q2VL32
C	505	HIS	-	expression tag	UNP Q2VL32
D	498	LEU	-	expression tag	UNP Q2VL32
D	499	GLU	-	expression tag	UNP Q2VL32
D	500	HIS	-	expression tag	UNP Q2VL32
D	501	HIS	-	expression tag	UNP Q2VL32
D	502	HIS	-	expression tag	UNP Q2VL32
D	503	HIS	-	expression tag	UNP Q2VL32
D	504	HIS	-	expression tag	UNP Q2VL32
D	505	HIS	-	expression tag	UNP Q2VL32

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ni 1 1	0	0
3	C	1	Total Ni 1 1	0	0
3	D	2	Total Ni 2 2	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

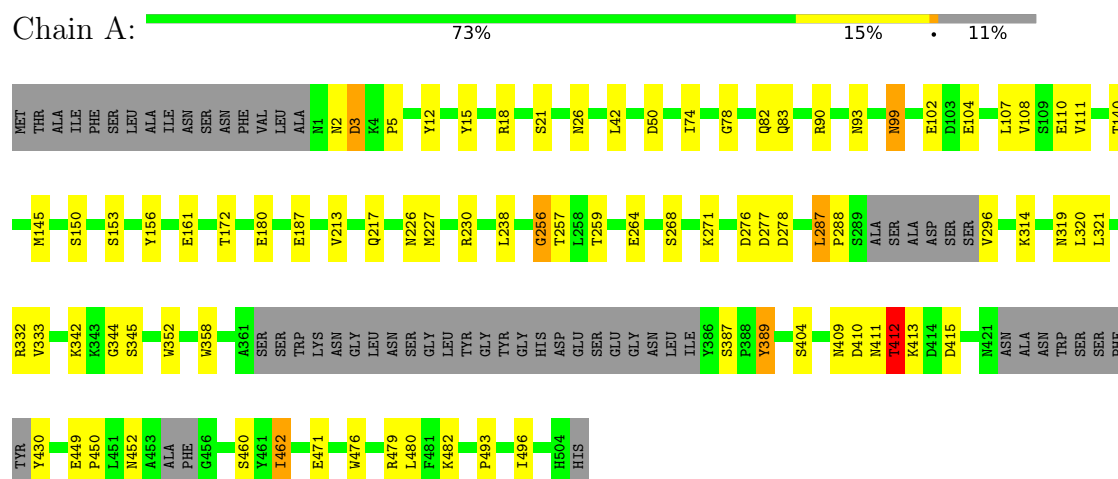
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	65	Total	O	0	0
			65	65		
5	B	69	Total	O	0	0
			69	69		
5	C	43	Total	O	0	0
			43	43		
5	D	30	Total	O	0	0
			30	30		

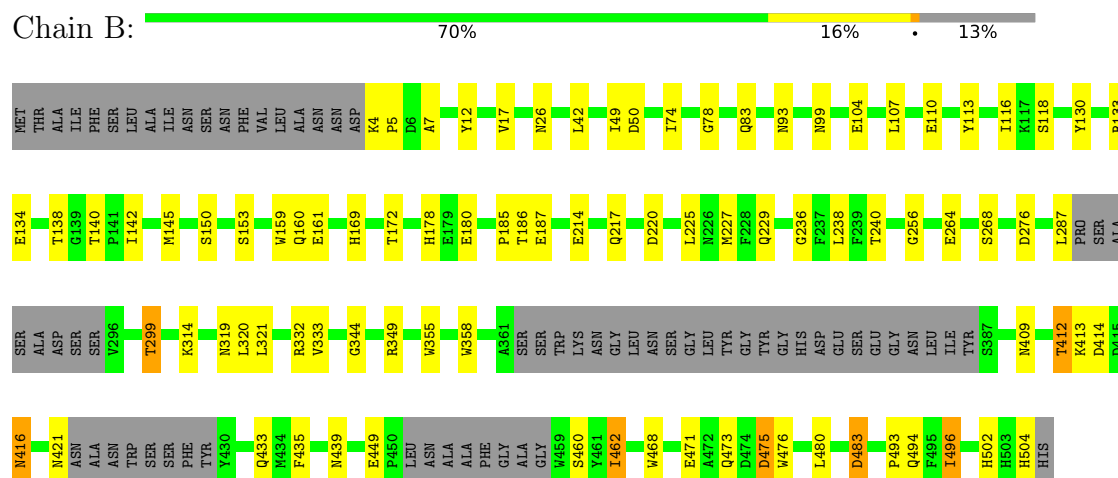
3 Residue-property plots

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: Aip56

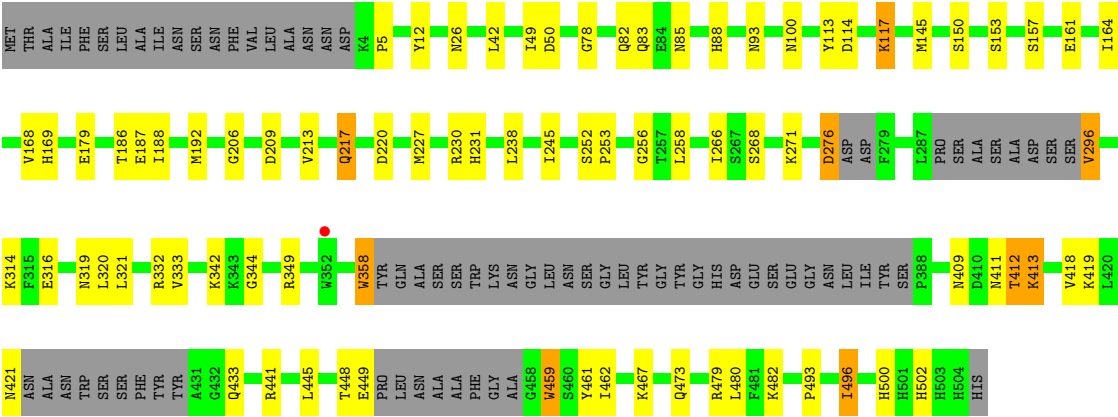


• Molecule 1: Aip56

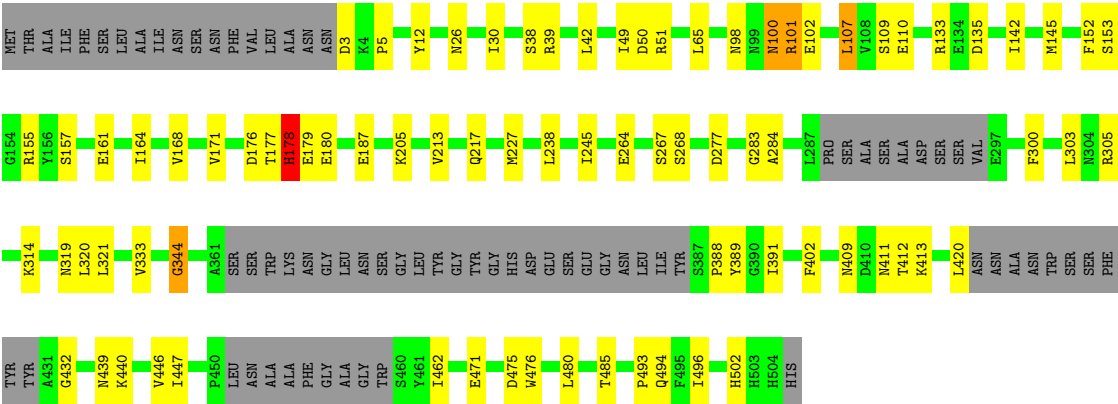


• Molecule 1: Aip56





● Molecule 1: Aip56



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.13Å 193.85Å 91.62Å 90.00° 113.24° 90.00°	Depositor
Resolution (Å)	46.28 – 2.54 46.28 – 2.54	Depositor EDS
% Data completeness (in resolution range)	69.6 (46.28-2.54) 69.4 (46.28-2.54)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.54Å)	Xtriage
Refinement program	BUSTER 2.10.4, PHENIX 1.20	Depositor
R, R_{free}	0.240 , 0.282 0.236 , 0.288	Depositor DCC
R_{free} test set	2563 reflections (3.37%)	wwPDB-VP
Wilson B-factor (Å ²)	49.4	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.125 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14880	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.38% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI, ZN, 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	0.79	0/3850	1.18	10/5221 (0.2%)
1	B	0.77	1/3765 (0.0%)	1.17	8/5104 (0.2%)
1	C	0.76	2/3698 (0.1%)	1.18	5/5008 (0.1%)
1	D	0.77	0/3729	1.21	10/5053 (0.2%)
All	All	0.77	3/15042 (0.0%)	1.19	33/20386 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	433	GLN	CA-C	5.65	1.59	1.52
1	C	448	THR	CA-C	5.27	1.58	1.53
1	B	433	GLN	CA-C	5.22	1.59	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	412	THR	CA-C-N	7.28	130.04	120.28
1	A	412	THR	C-N-CA	7.28	130.04	120.28
1	B	483	ASP	CA-CB-CG	6.71	119.31	112.60
1	A	26	ASN	CA-CB-CG	6.53	119.12	112.60
1	B	26	ASN	CA-CB-CG	6.33	118.93	112.60
1	D	26	ASN	CA-CB-CG	6.16	118.76	112.60
1	B	50	ASP	CA-CB-CG	5.87	118.47	112.60
1	A	50	ASP	CA-CB-CG	5.86	118.46	112.60
1	C	26	ASN	CA-CB-CG	5.84	118.44	112.60
1	A	93	ASN	CA-CB-CG	5.56	118.16	112.60
1	C	50	ASP	CA-CB-CG	5.53	118.13	112.60
1	D	178	HIS	CA-C-N	5.52	130.26	122.09
1	D	178	HIS	C-N-CA	5.52	130.26	122.09
1	D	50	ASP	CA-CB-CG	5.51	118.11	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	496	ILE	CA-C-N	5.50	127.66	120.28
1	B	496	ILE	C-N-CA	5.50	127.66	120.28
1	A	226	ASN	CA-CB-CG	5.39	117.99	112.60
1	C	276	ASP	CA-CB-CG	5.35	117.95	112.60
1	D	177	THR	CA-C-N	5.32	131.71	122.56
1	D	177	THR	C-N-CA	5.32	131.71	122.56
1	B	349	ARG	N-CA-C	5.23	117.19	107.99
1	A	496	ILE	CA-C-N	5.22	127.27	120.28
1	A	496	ILE	C-N-CA	5.22	127.27	120.28
1	D	3	ASP	CA-C-N	5.18	128.02	120.51
1	D	3	ASP	C-N-CA	5.18	128.02	120.51
1	C	217	GLN	CA-C-N	5.13	127.42	120.44
1	C	217	GLN	C-N-CA	5.13	127.42	120.44
1	A	278	ASP	CA-CB-CG	5.12	117.72	112.60
1	D	38	SER	CA-C-N	5.11	127.39	120.44
1	D	38	SER	C-N-CA	5.11	127.39	120.44
1	A	99	ASN	CA-CB-CG	5.09	117.69	112.60
1	B	217	GLN	CA-C-N	5.00	127.24	120.44
1	B	217	GLN	C-N-CA	5.00	127.24	120.44

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	3745	0	3519	46	0
1	B	3662	0	3446	50	0
1	C	3599	0	3398	42	0
1	D	3629	0	3416	38	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	2	0	0	0	0
4	A	6	0	8	1	0
4	B	24	0	32	3	0
5	A	65	0	0	1	0
5	B	69	0	0	2	0
5	C	43	0	0	1	0
5	D	30	0	0	2	0
All	All	14880	0	13819	166	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 6.

All (166) 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:B:462:ILE:HD13	1:B:471:GLU:HG3	1.62	0.81
1:A:332:ARG:HB2	5:A:701:HOH:O	1.82	0.78
1:B:138:THR:OG1	1:B:140:THR:HG22	1.85	0.77
1:A:476:TRP:HA	1:A:479:ARG:HG3	1.67	0.77
1:A:389:TYR:H	1:A:389:TYR:HD2	1.33	0.76
1:D:496:ILE:HD13	1:D:502:HIS:NE2	2.03	0.74
1:A:259:THR:CG2	1:B:240:THR:HG21	2.17	0.73
1:A:476:TRP:O	1:A:480:LEU:HB2	1.88	0.73
1:B:116:ILE:HG22	1:B:225:LEU:HD21	1.72	0.71
1:A:333:VAL:HG22	1:A:412:THR:HG23	1.75	0.69
1:C:231:HIS:ND1	1:C:238:LEU:HD13	2.07	0.68
1:B:160:GLN:HE22	4:B:604:GOL:H32	1.57	0.68
1:C:409:ASN:H	1:C:412:THR:HG22	1.59	0.68
1:C:459:TRP:CD1	1:C:459:TRP:N	2.61	0.67
1:B:409:ASN:H	1:B:412:THR:HG22	1.59	0.67
1:C:114:ASP:HA	1:C:117:LYS:HE2	1.77	0.67
1:A:259:THR:HG21	1:B:240:THR:HG21	1.78	0.66
1:B:220:ASP:HB3	5:B:722:HOH:O	1.95	0.66
1:B:496:ILE:HD13	1:B:502:HIS:NE2	2.12	0.65
1:D:471:GLU:HG2	1:D:476:TRP:HB3	1.81	0.63
1:D:176:ASP:OD1	5:D:701:HOH:O	2.15	0.63
1:A:409:ASN:H	1:A:412:THR:HG22	1.64	0.61
1:A:449:GLU:HB2	1:A:450:PRO:HD2	1.81	0.61
1:C:459:TRP:N	1:C:459:TRP:HD1	1.98	0.61
1:A:321:LEU:HD11	1:A:493:PRO:HB3	1.82	0.61
1:A:462:ILE:HD13	1:A:471:GLU:HG3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:LYS:NZ	1:C:419:LYS:HG2	2.16	0.60
1:B:113:TYR:H	4:B:603:GOL:H31	1.66	0.60
1:C:321:LEU:HD11	1:C:493:PRO:HB3	1.83	0.60
1:D:133:ARG:HG3	1:D:142:ILE:HB	1.84	0.60
1:D:314:LYS:HB3	1:D:320:LEU:HD23	1.84	0.60
1:C:413:LYS:HZ1	1:C:419:LYS:HG2	1.66	0.59
1:D:321:LEU:HD11	1:D:493:PRO:HB3	1.83	0.59
1:C:314:LYS:HB3	1:C:320:LEU:HD23	1.84	0.59
1:B:5:PRO:HG2	1:B:12:TYR:HA	1.85	0.59
1:B:321:LEU:HD11	1:B:493:PRO:HB3	1.84	0.59
1:C:473:GLN:HE22	1:C:479:ARG:HH22	1.51	0.59
1:A:257:THR:HA	1:B:240:THR:OG1	2.03	0.58
1:A:404:SER:HB3	1:A:430:TYR:HB2	1.86	0.58
1:C:473:GLN:NE2	1:C:479:ARG:HH22	2.02	0.58
1:A:2:ASN:ND2	1:A:18:ARG:NH1	2.52	0.57
1:A:314:LYS:HB3	1:A:320:LEU:HD23	1.86	0.57
1:B:416:ASN:HD22	1:B:468:TRP:H	1.53	0.56
1:B:460:SER:HB2	1:B:476:TRP:CH2	2.40	0.56
1:A:108:VAL:O	1:A:111:VAL:HG12	2.06	0.55
1:B:314:LYS:HB3	1:B:320:LEU:HD23	1.87	0.55
1:C:231:HIS:HE1	1:C:258:LEU:HD13	1.71	0.55
1:C:113:TYR:O	1:C:117:LYS:HG3	2.07	0.54
1:A:2:ASN:ND2	1:A:18:ARG:HH11	2.05	0.54
1:D:164:ILE:O	1:D:168:VAL:HG23	2.09	0.53
1:D:439:ASN:O	1:D:494:GLN:HG2	2.08	0.53
1:A:156:TYR:OH	4:A:603:GOL:O3	2.25	0.53
1:C:496:ILE:HD13	1:C:502:HIS:NE2	2.24	0.53
1:A:161:GLU:OE1	1:A:187:GLU:OE1	2.27	0.53
1:A:287:LEU:HD13	1:A:288:PRO:HD2	1.90	0.53
1:B:178:HIS:CD2	1:B:178:HIS:H	2.27	0.53
1:A:352:TRP:NE1	1:A:358:TRP:CE3	2.77	0.52
1:C:358:TRP:C	1:C:358:TRP:CD1	2.87	0.52
1:A:259:THR:HG23	1:B:240:THR:HG21	1.91	0.52
1:B:462:ILE:HD13	1:B:471:GLU:CG	2.38	0.52
1:B:169:HIS:CE1	1:B:186:THR:HG21	2.45	0.52
1:D:409:ASN:O	1:D:413:LYS:HB3	2.09	0.52
1:D:135:ASP:HB2	1:D:142:ILE:HD11	1.92	0.51
1:C:230:ARG:HG3	1:C:231:HIS:HD2	1.75	0.51
1:D:476:TRP:HB2	1:D:480:LEU:HD22	1.91	0.51
1:B:227:MET:SD	1:B:238:LEU:HD21	2.51	0.51
1:B:287:LEU:HD23	1:B:299:THR:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:TRP:CD1	1:A:358:TRP:HE3	2.29	0.51
1:D:107:LEU:HD23	1:D:110:GLU:HG3	1.93	0.51
1:B:160:GLN:NE2	4:B:604:GOL:H32	2.25	0.50
1:A:462:ILE:HD11	1:A:476:TRP:CD2	2.46	0.50
1:D:284:ALA:HB2	1:D:305:ARG:HH11	1.76	0.50
1:D:51:ARG:NH2	1:D:300:PHE:CE1	2.80	0.50
1:A:227:MET:SD	1:A:238:LEU:HD21	2.53	0.49
1:A:476:TRP:HA	1:A:479:ARG:HE	1.77	0.49
1:A:107:LEU:HB2	1:A:110:GLU:HG3	1.95	0.49
1:B:118:SER:HB3	1:D:267:SER:HB3	1.95	0.49
1:D:333:VAL:HG22	1:D:412:THR:CG2	2.43	0.49
1:B:225:LEU:HB3	1:D:152:PHE:HB3	1.95	0.48
1:D:51:ARG:NH2	1:D:300:PHE:HE1	2.11	0.48
1:A:99:ASN:ND2	1:A:102:GLU:OE2	2.46	0.48
1:A:352:TRP:NE1	1:A:358:TRP:HE3	2.12	0.48
1:B:355:TRP:HB2	1:B:435:PHE:CD2	2.49	0.48
1:D:5:PRO:HG2	1:D:12:TYR:HA	1.95	0.48
1:D:178:HIS:H	1:D:178:HIS:CD2	2.30	0.48
1:B:502:HIS:HD2	5:B:719:HOH:O	1.96	0.48
1:C:266:ILE:HG12	1:C:296:VAL:HG11	1.96	0.48
1:C:413:LYS:NZ	1:C:419:LYS:CG	2.77	0.48
1:A:256:GLY:HA3	1:B:236:GLY:HA3	1.96	0.48
1:C:231:HIS:CE1	1:C:238:LEU:HD13	2.49	0.48
1:D:409:ASN:HB3	1:D:412:THR:HB	1.96	0.47
1:D:321:LEU:CD1	1:D:493:PRO:HB3	2.44	0.47
1:A:476:TRP:HA	1:A:479:ARG:CG	2.42	0.47
1:C:164:ILE:O	1:C:168:VAL:HG23	2.13	0.47
1:C:227:MET:SD	1:C:238:LEU:HD21	2.54	0.47
1:B:321:LEU:CD1	1:B:493:PRO:HB3	2.44	0.47
1:A:150:SER:HB3	1:A:153:SER:HB3	1.97	0.47
1:D:161:GLU:OE2	1:D:187:GLU:OE2	2.32	0.47
1:A:321:LEU:CD1	1:A:493:PRO:HB3	2.43	0.47
1:B:225:LEU:HD13	1:D:152:PHE:CG	2.49	0.47
1:C:321:LEU:CD1	1:C:493:PRO:HB3	2.44	0.47
1:B:150:SER:HB3	1:B:153:SER:HB3	1.96	0.47
1:D:440:LYS:HG2	1:D:496:ILE:HA	1.98	0.46
1:D:227:MET:SD	1:D:238:LEU:HD21	2.55	0.46
1:B:333:VAL:HG22	1:B:412:THR:HG23	1.98	0.46
1:B:229:GLN:HG3	1:D:153:SER:HA	1.96	0.45
1:C:188:ILE:O	1:C:192:MET:HG3	2.17	0.45
1:B:4:LYS:N	1:B:5:PRO:HD3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:HIS:CE1	1:C:186:THR:HG21	2.52	0.45
1:D:344:GLY:HA3	1:D:388:PRO:HD2	1.99	0.45
1:D:391:ILE:HD13	5:D:702:HOH:O	2.17	0.45
1:B:138:THR:HG1	1:B:140:THR:HG22	1.81	0.44
1:C:413:LYS:HZ1	1:C:419:LYS:CG	2.30	0.44
1:D:333:VAL:HG22	1:D:412:THR:HG22	2.00	0.44
1:D:213:VAL:O	1:D:217:GLN:HG3	2.18	0.44
1:A:213:VAL:O	1:A:217:GLN:HG3	2.17	0.44
1:A:74:ILE:HG23	1:A:172:THR:CG2	2.48	0.44
1:B:107:LEU:HB2	1:B:110:GLU:HG3	2.00	0.44
1:A:345:SER:OG	1:A:387:SER:HB2	2.18	0.44
1:A:5:PRO:HG2	1:A:12:TYR:HA	2.00	0.43
1:B:74:ILE:HG23	1:B:172:THR:CG2	2.49	0.43
1:C:220:ASP:HB3	5:C:711:HOH:O	2.18	0.43
1:C:5:PRO:HG2	1:C:12:TYR:HA	2.00	0.43
1:B:332:ARG:CZ	1:B:414:ASP:HB2	2.49	0.43
1:B:473:GLN:HB3	1:B:475:ASP:OD2	2.18	0.43
1:C:161:GLU:OE1	1:C:187:GLU:OE2	2.36	0.43
1:B:130:TYR:HH	1:B:159:TRP:CD1	2.37	0.42
1:D:107:LEU:HD21	1:D:109:SER:HB2	2.00	0.42
1:B:439:ASN:O	1:B:494:GLN:HG2	2.19	0.42
1:A:389:TYR:HD2	1:A:389:TYR:N	2.08	0.42
1:B:161:GLU:OE2	1:B:187:GLU:OE2	2.37	0.42
1:C:150:SER:HB3	1:C:153:SER:HB3	2.01	0.42
1:C:213:VAL:O	1:C:217:GLN:HG3	2.19	0.42
1:C:413:LYS:HG2	1:C:418:VAL:HG11	2.02	0.42
1:D:402:PHE:HB3	1:D:432:GLY:O	2.20	0.42
1:B:7:ALA:O	1:B:185:PRO:HG3	2.19	0.42
1:B:358:TRP:CD1	1:B:435:PHE:HE2	2.37	0.42
1:B:78:GLY:HA2	1:B:83:GLN:HB2	2.01	0.42
1:C:206:GLY:H	1:C:209:ASP:HB2	1.85	0.42
1:D:98:ASN:HB3	1:D:101:ARG:HG2	2.01	0.42
1:A:352:TRP:CD1	1:A:358:TRP:CE3	3.07	0.42
1:C:49:ILE:HD13	1:C:245:ILE:HD12	2.02	0.42
1:C:252:SER:HA	1:C:253:PRO:HD3	1.97	0.42
1:B:49:ILE:HG13	1:B:93:ASN:CB	2.50	0.42
1:C:78:GLY:HA2	1:C:83:GLN:HB2	2.01	0.42
1:D:30:ILE:HG23	1:D:65:LEU:HG	2.02	0.41
1:D:49:ILE:HD13	1:D:245:ILE:HD12	2.02	0.41
1:C:85:ASN:HB3	1:C:88:HIS:CG	2.56	0.41
1:D:100:ASN:HB2	1:D:101:ARG:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:GLU:OE1	1:C:441:ARG:NH2	2.54	0.41
1:A:3:ASP:O	1:A:5:PRO:HD3	2.20	0.41
1:B:133:ARG:HG2	1:B:134:GLU:N	2.35	0.41
1:C:333:VAL:HG22	1:C:412:THR:HG23	2.02	0.41
1:A:140:THR:HG22	1:C:500:HIS:ND1	2.35	0.41
1:C:49:ILE:HG12	1:C:93:ASN:CB	2.51	0.41
1:A:78:GLY:HA2	1:A:83:GLN:HB2	2.02	0.41
1:A:333:VAL:CG2	1:A:412:THR:HG23	2.48	0.41
1:B:4:LYS:N	1:B:5:PRO:CD	2.84	0.41
1:B:416:ASN:HD22	1:B:468:TRP:N	2.17	0.41
1:C:117:LYS:HG3	1:C:117:LYS:H	1.67	0.41
1:D:227:MET:HE3	1:D:227:MET:HB3	1.94	0.41
1:C:445:LEU:HD23	1:C:461:TYR:CD2	2.54	0.41
1:B:476:TRP:HB2	1:B:480:LEU:HD22	2.02	0.40
1:A:5:PRO:HD2	1:A:15:TYR:CD2	2.55	0.40
1:A:409:ASN:O	1:A:413:LYS:HB2	2.22	0.40
1:A:460:SER:CB	1:A:476:TRP:HE1	2.33	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	454/521 (87%)	427 (94%)	25 (6%)	2 (0%)	30	39
1	B	442/521 (85%)	420 (95%)	19 (4%)	3 (1%)	18	25
1	C	433/521 (83%)	408 (94%)	22 (5%)	3 (1%)	18	25
1	D	439/521 (84%)	414 (94%)	23 (5%)	2 (0%)	24	34
All	All	1768/2084 (85%)	1669 (94%)	89 (5%)	10 (1%)	21	29

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	256	GLY
1	D	283	GLY
1	A	256	GLY
1	B	344	GLY
1	B	416	ASN
1	A	344	GLY
1	C	496	ILE
1	B	256	GLY
1	C	344	GLY
1	D	344	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	403/448 (90%)	377 (94%)	26 (6%)	15	22
1	B	395/448 (88%)	374 (95%)	21 (5%)	20	31
1	C	388/448 (87%)	362 (93%)	26 (7%)	15	21
1	D	392/448 (88%)	365 (93%)	27 (7%)	14	20
All	All	1578/1792 (88%)	1478 (94%)	100 (6%)	16	23

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	21	SER
1	A	42	LEU
1	A	82	GLN
1	A	90	ARG
1	A	104	GLU
1	A	145	MET
1	A	180	GLU
1	A	230	ARG
1	A	264	GLU
1	A	268	SER
1	A	271	LYS

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Mol	Chain	Res	Type
1	A	276	ASP
1	A	277	ASP
1	A	287	LEU
1	A	296	VAL
1	A	319	ASN
1	A	342	LYS
1	A	389	TYR
1	A	410	ASP
1	A	411	ASN
1	A	412	THR
1	A	415	ASP
1	A	452	ASN
1	A	462	ILE
1	A	482	LYS
1	B	17	VAL
1	B	42	LEU
1	B	99	ASN
1	B	104	GLU
1	B	142	ILE
1	B	145	MET
1	B	180	GLU
1	B	214	GLU
1	B	264	GLU
1	B	268	SER
1	B	276	ASP
1	B	299	THR
1	B	319	ASN
1	B	412	THR
1	B	413	LYS
1	B	421	ASN
1	B	449	GLU
1	B	462	ILE
1	B	475	ASP
1	B	483	ASP
1	B	504	HIS
1	C	42	LEU
1	C	82	GLN
1	C	100	ASN
1	C	117	LYS
1	C	145	MET
1	C	157	SER
1	C	179	GLU

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Mol	Chain	Res	Type
1	C	268	SER
1	C	271	LYS
1	C	276	ASP
1	C	296	VAL
1	C	319	ASN
1	C	332	ARG
1	C	342	LYS
1	C	349	ARG
1	C	358	TRP
1	C	411	ASN
1	C	412	THR
1	C	413	LYS
1	C	421	ASN
1	C	449	GLU
1	C	459	TRP
1	C	462	ILE
1	C	467	LYS
1	C	480	LEU
1	C	482	LYS
1	D	39	ARG
1	D	42	LEU
1	D	100	ASN
1	D	101	ARG
1	D	102	GLU
1	D	107	LEU
1	D	145	MET
1	D	155	ARG
1	D	157	SER
1	D	171	VAL
1	D	178	HIS
1	D	179	GLU
1	D	180	GLU
1	D	205	LYS
1	D	264	GLU
1	D	268	SER
1	D	277	ASP
1	D	303	LEU
1	D	319	ASN
1	D	389	TYR
1	D	411	ASN
1	D	420	LEU
1	D	446	VAL

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Mol	Chain	Res	Type
1	D	447	ILE
1	D	462	ILE
1	D	475	ASP
1	D	485	THR

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	2	ASN
1	A	181	ASN
1	A	183	GLN
1	A	421	ASN
1	A	439	ASN
1	A	501	HIS
1	B	73	HIS
1	B	122	GLN
1	B	178	HIS
1	B	181	ASN
1	B	183	GLN
1	B	416	ASN
1	B	439	ASN
1	B	478	GLN
1	B	494	GLN
1	C	122	GLN
1	C	123	GLN
1	C	178	HIS
1	C	181	ASN
1	C	183	GLN
1	C	229	GLN
1	C	231	HIS
1	C	421	ASN
1	C	439	ASN
1	C	473	GLN
1	C	501	HIS
1	D	80	HIS
1	D	178	HIS
1	D	181	ASN
1	D	183	GLN
1	D	217	GLN
1	D	229	GLN
1	D	330	ASN
1	D	411	ASN

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Mol	Chain	Res	Type
1	D	439	ASN
1	D	478	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 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	$\# Z > 2$
4	GOL	A	603	-	5,5,5	0.29	0	5,5,5	0.43	0
4	GOL	B	604	-	5,5,5	0.15	0	5,5,5	0.31	0
4	GOL	B	602	-	5,5,5	0.11	0	5,5,5	0.20	0
4	GOL	B	603	-	5,5,5	0.09	0	5,5,5	0.27	0
4	GOL	B	605	-	5,5,5	0.11	0	5,5,5	0.20	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
4	GOL	A	603	-	-	2/4/4/4	-
4	GOL	B	604	-	-	2/4/4/4	-
4	GOL	B	602	-	-	1/4/4/4	-
4	GOL	B	603	-	-	2/4/4/4	-
4	GOL	B	605	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	GOL	O1-C1-C2-C3
4	B	603	GOL	O1-C1-C2-C3
4	B	604	GOL	C1-C2-C3-O3
4	B	604	GOL	O2-C2-C3-O3
4	A	603	GOL	O1-C1-C2-O2
4	B	602	GOL	C1-C2-C3-O3
4	B	603	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	GOL	1	0
4	B	604	GOL	2	0
4	B	603	GOL	1	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 [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	464/521 (89%)	-1.12	0	100 100	25, 56, 88, 109	0
1	B	452/521 (86%)	-1.18	0	100 100	24, 56, 87, 98	0
1	C	445/521 (85%)	-0.63	1 (0%)	91 93	37, 76, 126, 142	0
1	D	449/521 (86%)	-0.90	0	100 100	30, 66, 109, 117	0
All	All	1810/2084 (86%)	-0.96	1 (0%)	92 94	24, 62, 110, 142	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	352	TRP	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](#)

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
4	GOL	B	605	6/6	0.96	0.08	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	B	604	6/6	0.98	0.04	54,55,55,55	0
4	GOL	B	603	6/6	0.98	0.06	51,51,52,52	0
4	GOL	A	603	6/6	0.99	0.04	43,44,44,44	0
4	GOL	B	602	6/6	0.99	0.04	59,59,59,59	0
2	ZN	B	601	1/1	0.99	0.01	40,40,40,40	0
2	ZN	D	601	1/1	0.99	0.01	44,44,44,44	0
3	NI	C	602	1/1	0.99	0.02	54,54,54,54	0
2	ZN	A	601	1/1	1.00	0.02	51,51,51,51	0
3	NI	A	602	1/1	1.00	0.01	38,38,38,38	0
2	ZN	C	601	1/1	1.00	0.01	50,50,50,50	0
3	NI	D	602	1/1	1.00	0.01	48,48,48,48	0
3	NI	D	603	1/1	1.00	0.01	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.