



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:08 PM UTC

PDB ID : 3T0J / pdb_00003t0j
Title : Crystal structure of inositol monophosphatase - II from Staphylococcus aureus
MSSA476
Authors : Dutta, A.; Bhattacharyya, S.; Dutta, D.; Das, A.K.
Deposited on : 2011-07-20
Resolution : 2.59 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

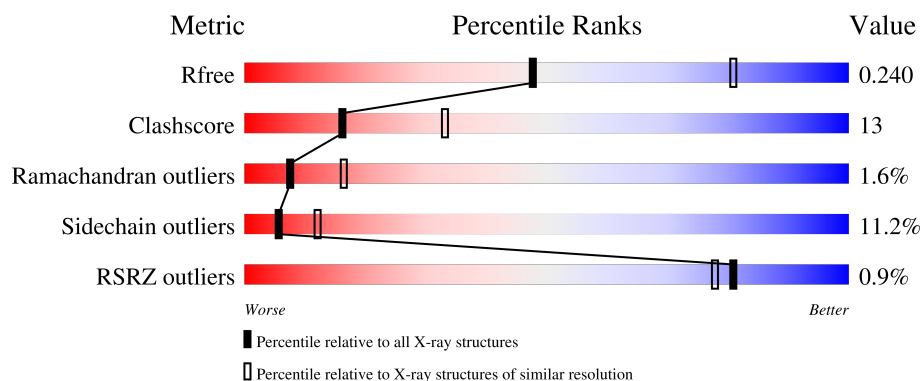
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	283	71% 18% • 6%
1	B	283	% 64% 20% 7% • 8%
1	C	283	% 69% 19% 6% 6%
1	D	283	% 64% 20% 7% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8500 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 Inositol monophosphatase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	1	0
			2070	1318	352	397	3			
1	B	260	Total	C	N	O	S	0	2	0
			2011	1280	337	390	4			
1	C	265	Total	C	N	O	S	0	0	0
			2050	1308	345	393	4			
1	D	257	Total	C	N	O	S	0	0	0
			1983	1262	332	385	4			

There are 32 discrepancies between the modelled and reference sequences:

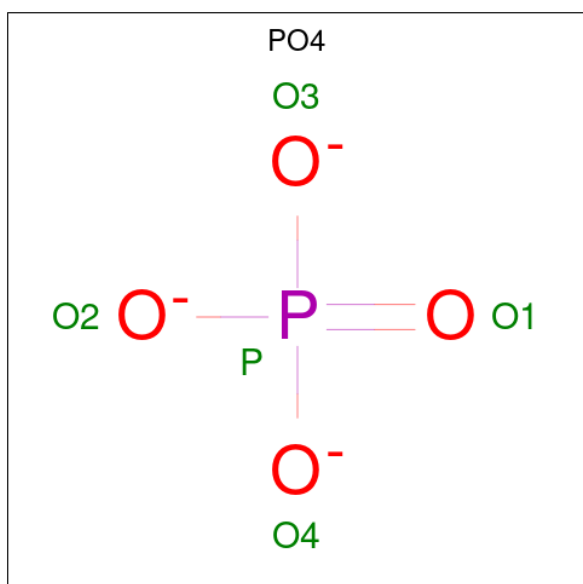
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	HIS	-	expression tag	UNP Q6GAA7
A	-6	HIS	-	expression tag	UNP Q6GAA7
A	-5	HIS	-	expression tag	UNP Q6GAA7
A	-4	HIS	-	expression tag	UNP Q6GAA7
A	-3	HIS	-	expression tag	UNP Q6GAA7
A	-2	HIS	-	expression tag	UNP Q6GAA7
A	-1	GLY	-	expression tag	UNP Q6GAA7
A	0	SER	-	expression tag	UNP Q6GAA7
B	-7	HIS	-	expression tag	UNP Q6GAA7
B	-6	HIS	-	expression tag	UNP Q6GAA7
B	-5	HIS	-	expression tag	UNP Q6GAA7
B	-4	HIS	-	expression tag	UNP Q6GAA7
B	-3	HIS	-	expression tag	UNP Q6GAA7
B	-2	HIS	-	expression tag	UNP Q6GAA7
B	-1	GLY	-	expression tag	UNP Q6GAA7
B	0	SER	-	expression tag	UNP Q6GAA7
C	-7	HIS	-	expression tag	UNP Q6GAA7
C	-6	HIS	-	expression tag	UNP Q6GAA7
C	-5	HIS	-	expression tag	UNP Q6GAA7
C	-4	HIS	-	expression tag	UNP Q6GAA7
C	-3	HIS	-	expression tag	UNP Q6GAA7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	HIS	-	expression tag	UNP Q6GAA7
C	-1	GLY	-	expression tag	UNP Q6GAA7
C	0	SER	-	expression tag	UNP Q6GAA7
D	-7	HIS	-	expression tag	UNP Q6GAA7
D	-6	HIS	-	expression tag	UNP Q6GAA7
D	-5	HIS	-	expression tag	UNP Q6GAA7
D	-4	HIS	-	expression tag	UNP Q6GAA7
D	-3	HIS	-	expression tag	UNP Q6GAA7
D	-2	HIS	-	expression tag	UNP Q6GAA7
D	-1	GLY	-	expression tag	UNP Q6GAA7
D	0	SER	-	expression tag	UNP Q6GAA7

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

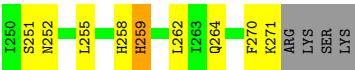
- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



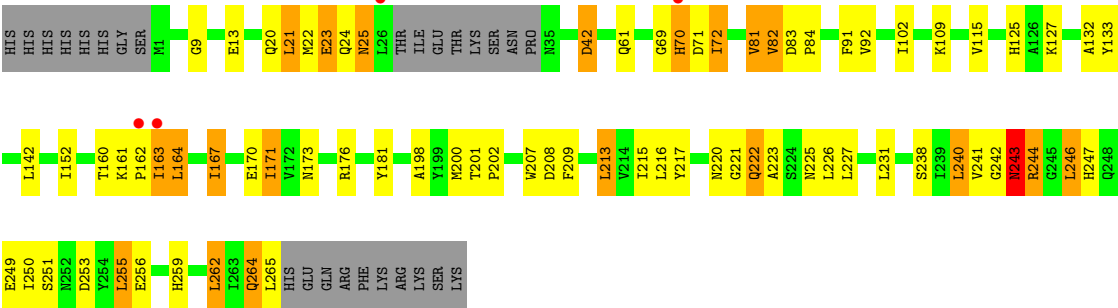
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		
3	A	1	Total	C	O	0	0
			13	8	5		
3	A	1	Total	C	O	0	0
			13	8	5		
3	B	1	Total	C	O	0	0
			10	6	4		
3	D	1	Total	C	O	0	0
			10	6	4		
3	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	81	Total	O	0	0
			81	81		
4	B	70	Total	O	0	0
			70	70		
4	C	76	Total	O	0	0
			76	76		
4	D	67	Total	O	0	0
			67	67		



● Molecule 1: Inositol monophosphatase family protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	179.14Å 55.21Å 149.47Å 90.00° 124.33° 90.00°	Depositor
Resolution (Å)	19.74 – 2.59 19.74 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.74-2.59) 99.4 (19.74-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.183 , 0.268 (Not available) , 0.240	Depositor DCC
R_{free} test set	1899 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.869	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8500	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.53% 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: PG4, PO4

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	0.91	1/2118 (0.0%)	1.07	7/2880 (0.2%)
1	B	0.92	0/2057	1.10	7/2800 (0.2%)
1	C	0.87	0/2095	1.11	7/2849 (0.2%)
1	D	0.87	1/2026 (0.0%)	1.08	0/2759
All	All	0.89	2/8296 (0.0%)	1.09	21/11288 (0.2%)

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	2
1	C	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	210	ALA	CA-CB	-5.36	1.45	1.53
1	D	92	VAL	CA-CB	5.20	1.60	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	ASN	N-CA-C	-7.13	103.84	112.54
1	B	171	ILE	CB-CA-C	6.91	121.47	112.14
1	C	252	ASN	N-CA-C	6.90	121.94	112.90
1	A	81	VAL	CB-CA-C	5.55	118.21	110.99
1	A	171	ILE	N-CA-C	5.50	117.00	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	GLY	CA-C-N	-5.41	114.19	122.62
1	A	221	GLY	C-N-CA	-5.41	114.19	122.62
1	C	235	GLY	CA-C-N	5.39	125.69	119.92
1	C	235	GLY	C-N-CA	5.39	125.69	119.92
1	A	85	ILE	N-CA-C	5.30	114.42	106.42
1	B	140	LYS	CA-C-N	5.23	125.23	119.90
1	B	140	LYS	C-N-CA	5.23	125.23	119.90
1	B	72	ILE	N-CA-C	5.18	117.00	108.97
1	B	252	ASN	CA-C-N	-5.10	114.58	122.49
1	B	252	ASN	C-N-CA	-5.10	114.58	122.49
1	C	42	ASP	N-CA-C	-5.08	105.43	110.97
1	C	102	ILE	CA-C-N	-5.05	118.64	122.33
1	C	102	ILE	C-N-CA	-5.05	118.64	122.33
1	C	264	GLN	N-CA-C	-5.05	105.05	111.11
1	A	222	GLN	N-CA-C	5.04	117.46	109.50
1	B	261	ALA	N-CA-C	-5.03	100.09	110.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	271	LYS	Peptide
1	A	34	PRO	Peptide
1	C	245	GLY	Peptide

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	2070	0	2007	39	0
1	B	2011	0	1955	65	0
1	C	2050	0	1989	55	0
1	D	1983	0	1917	56	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	39	0	54	10	0
3	B	10	0	13	2	0
3	D	23	0	31	2	0
4	A	81	0	0	3	0
4	B	70	0	0	2	0
4	C	76	0	0	3	0
4	D	67	0	0	2	0
All	All	8500	0	7966	211	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 13.

All (211) 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:C:1:MET:CE	1:C:127:LYS:HE2	1.81	1.09
1:C:1:MET:HE1	1:C:127:LYS:CE	1.88	1.03
1:B:261:ALA:O	1:B:263:ILE:N	1.99	0.94
1:A:155:ASN:HD22	1:A:157:ASN:H	1.12	0.93
1:A:70:HIS:O	1:A:71:ASP:HB2	1.66	0.92
1:C:1:MET:HE1	1:C:127:LYS:HE2	0.93	0.92
1:B:237[A]:ASN:N	1:B:237[A]:ASN:HD22	1.66	0.89
1:B:12:GLN:HE22	1:C:12:GLN:HE22	1.13	0.89
1:B:264:GLN:HE21	1:B:264:GLN:N	1.72	0.87
1:A:155:ASN:ND2	1:A:157:ASN:H	1.76	0.83
1:C:193:THR:CG2	1:C:195:ASN:HB2	2.09	0.82
1:C:160:THR:HG21	1:D:173:ASN:OD1	1.81	0.80
1:B:237[A]:ASN:N	1:B:237[A]:ASN:ND2	2.27	0.78
1:D:242:GLY:O	1:D:243:ASN:HB3	1.85	0.77
1:B:237[A]:ASN:HD22	1:B:237[A]:ASN:H	1.35	0.75
1:D:22:MET:O	1:D:23:GLU:HG2	1.88	0.73
1:D:69:GLY:HA2	1:D:72:ILE:CD1	2.18	0.73
1:D:163:ILE:O	1:D:164:LEU:HB2	1.88	0.73
1:C:193:THR:HG22	1:C:195:ASN:HB2	1.70	0.72
1:A:271:LYS:HG3	1:A:272:ARG:HA	1.72	0.72
1:D:71:ASP:O	1:D:72:ILE:C	2.33	0.71
1:B:152:ILE:HD13	1:B:171:ILE:CD1	2.21	0.70
1:A:134:ARG:HE	3:A:277:PG4:H32	1.57	0.69
1:B:171:ILE:HD13	1:B:171:ILE:C	2.17	0.69
1:C:222:GLN:HG3	1:C:244:ARG:HG2	1.74	0.69
1:C:226:LEU:HG	1:C:238:SER:HB2	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:GLY:HA2	1:C:248:GLN:H	1.58	0.68
1:C:157:ASN:O	1:C:160:THR:HB	1.93	0.68
1:C:209:PHE:O	1:C:213:LEU:HB2	1.94	0.67
1:A:46:GLU:OE2	1:A:68:HIS:HD2	1.77	0.67
1:D:244:ARG:HG2	4:D:299:HOH:O	1.96	0.65
1:D:213:LEU:O	1:D:217:TYR:HD2	1.78	0.64
1:A:70:HIS:O	1:A:71:ASP:CB	2.41	0.64
1:D:69:GLY:HA2	1:D:72:ILE:HD11	1.80	0.64
1:D:198:ALA:HB2	1:D:246:LEU:HD21	1.81	0.63
1:A:156:PRO:HD3	1:B:156:PRO:HG3	1.82	0.62
1:C:10:LEU:HD11	1:C:49:ILE:HG23	1.82	0.61
1:D:216:LEU:HG	1:D:221:GLY:HA3	1.83	0.61
1:B:225:ASN:HB2	1:B:238[B]:SER:OG	2.00	0.61
1:D:81:VAL:HG23	1:D:207:TRP:HA	1.82	0.61
1:D:81:VAL:CG2	1:D:207:TRP:HA	2.32	0.60
1:D:42:ASP:OD2	1:D:84:PRO:HG2	2.01	0.60
1:B:196:LEU:O	4:B:301:HOH:O	2.17	0.60
1:B:152:ILE:HD13	1:B:171:ILE:HD11	1.84	0.59
1:A:182:GLY:O	3:A:279:PG4:H61	2.03	0.59
1:D:264:GLN:HA	1:D:264:GLN:HE21	1.68	0.58
1:B:24:GLN:O	1:B:24:GLN:HG3	2.02	0.58
1:C:193:THR:HG22	1:C:195:ASN:H	1.67	0.58
1:D:69:GLY:HA2	1:D:72:ILE:HD12	1.85	0.58
1:D:70:HIS:C	1:D:72:ILE:H	2.11	0.58
1:D:244:ARG:CG	4:D:299:HOH:O	2.52	0.58
1:D:249:GLU:O	1:D:253:ASP:CB	2.52	0.58
1:B:198:ALA:HB2	1:B:246:LEU:HD21	1.86	0.58
1:B:81:VAL:HG12	1:B:103:GLY:O	2.04	0.57
1:D:9:GLY:O	1:D:13:GLU:HG3	2.04	0.57
1:D:22:MET:C	1:D:23:GLU:HG2	2.28	0.57
1:D:164:LEU:HA	1:D:167:ILE:HG12	1.86	0.56
1:A:209:PHE:HB2	1:A:213:LEU:HD13	1.86	0.56
1:B:65:GLU:OE1	1:B:66:GLU:OE2	2.23	0.56
1:D:21:LEU:C	1:D:23:GLU:H	2.12	0.56
1:B:159:LEU:HD21	1:B:172:VAL:HG11	1.88	0.56
1:B:226:LEU:HG	1:B:238[B]:SER:HB2	1.86	0.56
1:B:256:GLU:HG3	1:B:257:PRO:HD3	1.87	0.56
1:D:222:GLN:O	1:D:241:VAL:HA	2.05	0.56
1:B:81:VAL:HG22	1:B:207:TRP:HA	1.85	0.56
1:D:69:GLY:O	1:D:70:HIS:HB3	2.06	0.56
1:B:203:ARG:HG3	4:B:282:HOH:O	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:LEU:HG	1:B:238[A]:SER:HB3	1.87	0.56
1:D:264:GLN:O	1:D:265:LEU:CB	2.54	0.56
1:D:152:ILE:HD13	1:D:171:ILE:HD13	1.87	0.56
1:C:139:LEU:O	1:C:140:LYS:CB	2.54	0.55
1:C:245:GLY:HA2	1:C:248:GLN:N	2.22	0.55
1:C:82:VAL:HB	1:C:102:ILE:HG12	1.90	0.54
1:C:170:GLU:HA	1:C:170:GLU:OE1	2.08	0.54
1:C:244:ARG:O	1:C:245:GLY:O	2.26	0.54
1:A:134:ARG:HH21	3:A:277:PG4:H22	1.73	0.53
1:C:152:ILE:HG22	1:C:198:ALA:HB3	1.90	0.53
1:D:249:GLU:O	1:D:253:ASP:HB3	2.08	0.53
1:A:155:ASN:HD22	1:A:157:ASN:N	1.92	0.53
1:C:245:GLY:HA2	1:C:248:GLN:HB2	1.89	0.53
1:C:81:VAL:CG2	1:C:207:TRP:HA	2.39	0.52
1:A:271:LYS:HG3	1:A:272:ARG:CA	2.40	0.52
1:B:69:GLY:O	1:B:72:ILE:HG12	2.09	0.52
1:C:271:LYS:HA	4:C:306:HOH:O	2.09	0.52
1:D:83:ASP:OD2	1:D:208:ASP:OD1	2.26	0.52
1:D:251:SER:HA	1:D:255:LEU:HB2	1.90	0.52
1:D:125:HIS:CE1	1:D:133:TYR:HB2	2.45	0.52
1:B:155:ASN:OD1	1:B:157:ASN:HB2	2.11	0.51
1:A:269:ARG:HB2	3:A:278:PG4:H71	1.93	0.51
1:B:147:LEU:O	1:B:175:SER:HA	2.10	0.51
1:C:169:LYS:HB2	1:D:160:THR:HG22	1.91	0.51
1:B:33:ASN:N	1:B:34:PRO:HD2	2.26	0.51
1:C:160:THR:HG22	1:C:161:LYS:HD2	1.92	0.51
1:D:249:GLU:O	1:D:253:ASP:HB2	2.12	0.50
1:C:15:GLY:HA3	1:C:116:TYR:HE2	1.76	0.50
1:B:204:LEU:HD22	1:B:239:ILE:HG13	1.94	0.50
3:D:277:PG4:H51	3:D:278:PG4:H22	1.93	0.50
1:B:163:ILE:O	1:B:167:ILE:HG23	2.12	0.50
1:A:265:LEU:HD22	3:A:278:PG4:H81	1.93	0.50
1:B:263:ILE:C	1:B:264:GLN:HE21	2.20	0.50
1:B:153:GLY:HA2	1:B:179:ARG:O	2.11	0.49
1:A:83:ASP:HB2	1:A:207:TRP:HB2	1.94	0.49
1:B:243:ASN:ND2	1:B:246:LEU:H	2.10	0.49
1:D:226:LEU:HG	1:D:238:SER:HB2	1.95	0.49
1:B:171:ILE:HD13	1:B:171:ILE:O	2.12	0.49
1:D:82:VAL:HB	1:D:102:ILE:HG12	1.94	0.49
1:A:4:TYR:CE2	4:A:280:HOH:O	2.55	0.49
1:B:76:LYS:HD2	1:B:76:LYS:HA	1.64	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:PHE:C	1:D:91:PHE:CD2	2.90	0.49
1:B:91:PHE:C	1:B:91:PHE:CD2	2.91	0.48
1:A:163:ILE:HG22	1:A:265:LEU:HD11	1.94	0.48
1:B:9:GLY:HA3	1:C:5:GLY:O	2.13	0.48
3:A:279:PG4:H62	4:A:295:HOH:O	2.13	0.48
1:B:126:ALA:HB2	1:B:132:ALA:HA	1.97	0.47
1:B:34:PRO:HB2	1:B:92:VAL:HG13	1.97	0.47
1:D:223:ALA:HB1	1:D:231:LEU:HD12	1.94	0.47
1:A:155:ASN:HD22	1:A:155:ASN:C	2.23	0.47
1:A:226:LEU:HD12	1:A:238:SER:HB2	1.96	0.47
1:C:124:TYR:CE1	1:C:134:ARG:HG3	2.50	0.47
1:B:124:TYR:CE1	1:B:134:ARG:HG3	2.49	0.47
1:C:206:PRO:HA	1:C:209:PHE:CZ	2.50	0.47
1:C:251:SER:HA	1:C:255:LEU:HD12	1.97	0.47
1:C:139:LEU:HA	1:C:139:LEU:HD12	1.68	0.47
1:C:168:PHE:O	1:C:172:VAL:HG23	2.15	0.46
1:C:245:GLY:HA2	1:C:248:GLN:CB	2.44	0.46
1:B:134:ARG:HD2	3:B:277:PG4:O1	2.16	0.46
1:C:41:VAL:HG12	1:C:85:ILE:HD11	1.97	0.46
1:B:162:PRO:C	1:B:164:LEU:H	2.24	0.46
1:C:68:HIS:HE1	4:C:302:HOH:O	1.98	0.46
1:B:45:THR:HG22	1:B:84:PRO:HB3	1.97	0.45
1:D:152:ILE:HG22	1:D:198:ALA:HB3	1.99	0.45
1:D:181:TYR:CE2	3:D:278:PG4:H12	2.51	0.45
1:D:250:ILE:HG22	1:D:255:LEU:HD22	1.98	0.45
1:B:45:THR:CG2	1:B:84:PRO:HB3	2.47	0.45
1:A:116:TYR:HB2	1:A:123:LEU:HD13	1.99	0.45
1:B:170:GLU:OE1	1:B:170:GLU:HA	2.17	0.45
1:D:213:LEU:HG	1:D:217:TYR:HE2	1.82	0.45
1:A:134:ARG:HH21	3:A:277:PG4:C2	2.30	0.45
1:D:152:ILE:HA	1:D:198:ALA:O	2.17	0.45
1:A:46:GLU:OE2	1:A:68:HIS:CD2	2.65	0.44
1:C:140:LYS:HA	1:C:141:PRO:HD3	1.86	0.44
1:C:193:THR:HG22	1:C:195:ASN:CB	2.44	0.44
1:D:209:PHE:O	1:D:213:LEU:HB2	2.18	0.44
1:B:170:GLU:OE1	1:B:170:GLU:CA	2.66	0.44
1:D:200:MET:HE1	1:D:250:ILE:HD13	2.00	0.44
1:C:206:PRO:HA	1:C:209:PHE:CE2	2.52	0.44
1:D:167:ILE:HD13	1:D:262:LEU:HD13	1.98	0.44
1:B:11:ILE:HD12	1:B:102:ILE:HD12	1.98	0.44
1:D:227:LEU:HD21	1:D:262:LEU:HB3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:GLU:O	1:B:174:ASP:HB2	2.18	0.44
1:B:204:LEU:CD2	1:B:239:ILE:HG13	2.47	0.44
1:C:10:LEU:CD1	1:C:49:ILE:HG23	2.47	0.43
1:D:70:HIS:C	1:D:72:ILE:N	2.76	0.43
1:B:171:ILE:CD1	1:B:171:ILE:C	2.90	0.43
3:B:277:PG4:H62	3:B:277:PG4:H41	1.88	0.43
1:B:260:ASP:O	1:B:261:ALA:HB3	2.18	0.43
1:C:258:HIS:O	1:C:259:HIS:C	2.60	0.43
1:B:209:PHE:O	1:B:213:LEU:HB2	2.19	0.43
1:B:15:GLY:HA3	1:B:116:TYR:HE2	1.82	0.43
1:A:82:VAL:HB	1:A:102:ILE:HG12	2.00	0.43
1:B:191:VAL:HG21	1:B:241:VAL:HG23	2.01	0.43
1:C:45:THR:HB	1:C:84:PRO:HB3	2.00	0.43
1:C:134:ARG:HD2	4:C:338:HOH:O	2.18	0.43
1:C:245:GLY:CA	1:C:248:GLN:H	2.30	0.43
1:C:153:GLY:HA2	1:C:179:ARG:O	2.19	0.42
1:C:226:LEU:HG	1:C:238:SER:CB	2.46	0.42
1:A:124:TYR:CE1	1:A:134:ARG:HG3	2.54	0.42
1:B:170:GLU:HB3	1:B:254:TYR:CD2	2.54	0.42
1:C:246:LEU:H	1:C:249:GLU:H	1.67	0.42
1:B:225:ASN:HB2	1:B:238[A]:SER:HB2	1.99	0.42
1:A:259:HIS:HE1	4:A:308:HOH:O	2.02	0.42
1:B:164:LEU:HD12	1:B:164:LEU:HA	1.74	0.42
1:B:226:LEU:H	1:B:238[A]:SER:HB2	1.85	0.42
1:C:63:LEU:O	1:C:81:VAL:HA	2.19	0.42
1:C:91:PHE:CD2	1:C:91:PHE:C	2.97	0.42
1:D:163:ILE:HG22	1:D:164:LEU:N	2.35	0.42
1:B:258:HIS:O	1:B:260:ASP:O	2.38	0.42
1:C:213:LEU:HD11	1:C:231:LEU:HD12	2.02	0.42
1:D:167:ILE:HD13	1:D:262:LEU:CD1	2.49	0.42
1:C:209:PHE:HB2	1:C:213:LEU:HD13	2.02	0.42
1:A:186:LEU:HB3	3:A:277:PG4:H81	2.01	0.41
1:A:216:LEU:HD22	1:A:221:GLY:HA3	2.02	0.41
1:D:132:ALA:HB1	1:D:215:ILE:HG23	2.02	0.41
1:D:200:MET:HE2	1:D:200:MET:HB3	1.96	0.41
1:B:46:GLU:HG2	1:B:68:HIS:HD2	1.85	0.41
1:C:152:ILE:HD12	1:C:154:ILE:HG22	2.01	0.41
1:C:173:ASN:OD1	1:D:160:THR:HB	2.21	0.41
1:B:46:GLU:O	1:B:47:ASP:C	2.63	0.41
1:B:152:ILE:O	1:B:152:ILE:HG13	2.20	0.41
1:B:159:LEU:HD12	1:B:159:LEU:HA	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:PHE:C	1:C:271:LYS:HG2	2.44	0.41
1:A:125:HIS:NE2	1:A:135:GLY:O	2.53	0.41
1:A:127:LYS:HE3	1:A:130:GLU:OE2	2.19	0.41
1:A:154:ILE:HG23	1:A:154:ILE:O	2.20	0.41
1:D:69:GLY:O	1:D:70:HIS:CB	2.68	0.41
1:A:137:GLN:HA	1:A:138:PRO:HD2	1.94	0.41
1:A:164:LEU:HD21	1:A:202:PRO:HG3	2.02	0.41
1:C:144:ASP:HA	1:C:243:ASN:ND2	2.35	0.41
1:A:35:ASN:O	1:A:38:VAL:HG12	2.19	0.41
1:A:134:ARG:NH2	3:A:277:PG4:H22	2.35	0.41
1:B:12:GLN:HE22	1:C:12:GLN:NE2	1.97	0.41
1:D:201:THR:OG1	1:D:202:PRO:HD2	2.21	0.41
1:D:240:LEU:HD13	1:D:247:HIS:CD2	2.55	0.41
1:D:225:ASN:HB2	1:D:238:SER:OG	2.20	0.41
1:A:65:GLU:HA	1:A:207:TRP:CE2	2.55	0.40
1:A:171:ILE:HD11	1:A:200:MET:HE1	2.03	0.40
1:B:71:ASP:OD2	1:B:71:ASP:N	2.54	0.40
1:B:161:LYS:HA	1:B:162:PRO:HD2	1.86	0.40
1:A:84:PRO:O	1:A:100:ILE:HG12	2.21	0.40
1:A:203:ARG:HH11	1:A:203:ARG:HD3	1.75	0.40
3:A:279:PG4:H21	1:B:176:ARG:NH2	2.36	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	263/283 (93%)	251 (95%)	10 (4%)	2 (1%)	16	34
1	B	258/283 (91%)	245 (95%)	9 (4%)	4 (2%)	7	16
1	C	261/283 (92%)	244 (94%)	13 (5%)	4 (2%)	8	18
1	D	253/283 (89%)	229 (90%)	17 (7%)	7 (3%)	4	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1035/1132 (91%)	969 (94%)	49 (5%)	17 (2%)	7	16

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	262	LEU
1	C	246	LEU
1	D	70	HIS
1	A	71	ASP
1	B	261	ALA
1	C	245	GLY
1	D	24	GLN
1	D	72	ILE
1	D	162	PRO
1	D	243	ASN
1	A	26	LEU
1	B	263	ILE
1	C	140	LYS
1	D	25	ASN
1	D	164	LEU
1	C	54	LEU
1	B	163	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	218/239 (91%)	196 (90%)	22 (10%)	7	15
1	B	214/239 (90%)	189 (88%)	25 (12%)	5	11
1	C	216/239 (90%)	196 (91%)	20 (9%)	8	18
1	D	210/239 (88%)	180 (86%)	30 (14%)	3	6
All	All	858/956 (90%)	761 (89%)	97 (11%)	6	12

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	42	ASP
1	A	43	LYS
1	A	71	ASP
1	A	72	ILE
1	A	81	VAL
1	A	82	VAL
1	A	109	LYS
1	A	115	VAL
1	A	140	LYS
1	A	154	ILE
1	A	155	ASN
1	A	169	LYS
1	A	171	ILE
1	A	203	ARG
1	A	216	LEU
1	A	220	ASN
1	A	222	GLN
1	A	233	ILE
1	A	246	LEU
1	A	259	HIS
1	A	272	ARG
1	B	39	THR
1	B	71	ASP
1	B	76	LYS
1	B	82	VAL
1	B	115	VAL
1	B	157	ASN
1	B	159	LEU
1	B	160	THR
1	B	164	LEU
1	B	167	ILE
1	B	170	GLU
1	B	171	ILE
1	B	172	VAL
1	B	174	ASP
1	B	176	ARG
1	B	203	ARG
1	B	213	LEU
1	B	237[A]	ASN
1	B	237[B]	ASN
1	B	243	ASN
1	B	244	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	246	LEU
1	B	256	GLU
1	B	264	GLN
1	B	265	LEU
1	C	10	LEU
1	C	26	LEU
1	C	54	LEU
1	C	71	ASP
1	C	81	VAL
1	C	82	VAL
1	C	115	VAL
1	C	139	LEU
1	C	152	ILE
1	C	159	LEU
1	C	160	THR
1	C	170	GLU
1	C	171	ILE
1	C	193	THR
1	C	213	LEU
1	C	216	LEU
1	C	222	GLN
1	C	243	ASN
1	C	259	HIS
1	C	262	LEU
1	D	20	GLN
1	D	21	LEU
1	D	23	GLU
1	D	25	ASN
1	D	42	ASP
1	D	61	GLN
1	D	81	VAL
1	D	82	VAL
1	D	109	LYS
1	D	115	VAL
1	D	127	LYS
1	D	142	LEU
1	D	161	LYS
1	D	163	ILE
1	D	167	ILE
1	D	170	GLU
1	D	171	ILE
1	D	176	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	213	LEU
1	D	220	ASN
1	D	222	GLN
1	D	240	LEU
1	D	243	ASN
1	D	244	ARG
1	D	246	LEU
1	D	255	LEU
1	D	256	GLU
1	D	259	HIS
1	D	262	LEU
1	D	264	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	25	ASN
1	A	35	ASN
1	A	68	HIS
1	A	94	GLN
1	A	97	ASN
1	A	155	ASN
1	A	157	ASN
1	A	173	ASN
1	A	195	ASN
1	A	220	ASN
1	A	247	HIS
1	A	259	HIS
1	A	268	GLN
1	B	12	GLN
1	B	25	ASN
1	B	40	ASN
1	B	61	GLN
1	B	68	HIS
1	B	94	GLN
1	B	205	GLN
1	B	243	ASN
1	B	264	GLN
1	C	20	GLN
1	C	25	ASN
1	C	40	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	61	GLN
1	C	68	HIS
1	C	93	HIS
1	C	94	GLN
1	C	97	ASN
1	C	137	GLN
1	C	146	ASN
1	C	195	ASN
1	C	243	ASN
1	C	247	HIS
1	C	259	HIS
1	C	268	GLN
1	D	20	GLN
1	D	25	ASN
1	D	40	ASN
1	D	59	ASN
1	D	94	GLN
1	D	97	ASN
1	D	157	ASN
1	D	205	GLN
1	D	220	ASN
1	D	222	GLN
1	D	264	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](#)

10 ligands 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	$\# Z > 2$
3	PG4	D	278	-	12,12,12	0.58	0	11,11,11	0.65	0
3	PG4	D	277	-	9,9,12	0.61	0	8,8,11	0.28	0
3	PG4	A	277	-	12,12,12	0.55	0	11,11,11	0.25	0
2	PO4	A	276	-	4,4,4	1.42	0	6,6,6	1.04	0
2	PO4	C	276	-	4,4,4	0.72	0	6,6,6	0.99	0
3	PG4	B	277	-	9,9,12	0.56	0	8,8,11	0.35	0
2	PO4	B	276	-	4,4,4	1.13	0	6,6,6	0.82	0
2	PO4	D	276	-	4,4,4	0.68	0	6,6,6	0.83	0
3	PG4	A	278	-	12,12,12	0.70	0	11,11,11	0.47	0
3	PG4	A	279	-	12,12,12	0.56	0	11,11,11	0.45	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	PG4	D	278	-	-	5/10/10/10	-
3	PG4	D	277	-	-	4/7/7/10	-
3	PG4	A	277	-	-	6/10/10/10	-
3	PG4	A	278	-	-	6/10/10/10	-
3	PG4	B	277	-	-	6/7/7/10	-
3	PG4	A	279	-	-	3/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	277	PG4	O3-C5-C6-O4
3	B	277	PG4	O2-C3-C4-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	279	PG4	O3-C5-C6-O4
3	A	277	PG4	O1-C1-C2-O2
3	D	277	PG4	O1-C1-C2-O2
3	D	278	PG4	C5-C6-O4-C7
3	A	278	PG4	O2-C3-C4-O3
3	D	278	PG4	O2-C3-C4-O3
3	A	279	PG4	C6-C5-O3-C4
3	A	278	PG4	C8-C7-O4-C6
3	A	277	PG4	C4-C3-O2-C2
3	D	278	PG4	C8-C7-O4-C6
3	A	278	PG4	O4-C7-C8-O5
3	A	278	PG4	C6-C5-O3-C4
3	A	277	PG4	C6-C5-O3-C4
3	D	277	PG4	C1-C2-O2-C3
3	A	277	PG4	C3-C4-O3-C5
3	A	279	PG4	C4-C3-O2-C2
3	D	278	PG4	C6-C5-O3-C4
3	A	278	PG4	C5-C6-O4-C7
3	A	278	PG4	O1-C1-C2-O2
3	B	277	PG4	C1-C2-O2-C3
3	B	277	PG4	C6-C5-O3-C4
3	B	277	PG4	C3-C4-O3-C5
3	A	277	PG4	C1-C2-O2-C3
3	D	277	PG4	C3-C4-O3-C5
3	B	277	PG4	O1-C1-C2-O2
3	B	277	PG4	C4-C3-O2-C2
3	D	278	PG4	O1-C1-C2-O2
3	D	277	PG4	O2-C3-C4-O3

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	278	PG4	2	0
3	D	277	PG4	1	0
3	A	277	PG4	5	0
3	B	277	PG4	2	0
3	A	278	PG4	2	0
3	A	279	PG4	3	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	266/283 (93%)	-0.53	1 (0%) 88 86	12, 24, 45, 63	2 (0%)
1	B	260/283 (91%)	-0.46	2 (0%) 82 80	12, 25, 52, 75	3 (1%)
1	C	265/283 (93%)	-0.42	2 (0%) 82 80	16, 29, 47, 67	1 (0%)
1	D	257/283 (90%)	-0.25	4 (1%) 70 66	18, 32, 60, 74	1 (0%)
All	All	1048/1132 (92%)	-0.42	9 (0%) 81 78	12, 28, 54, 75	7 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	34	PRO	3.5
1	D	26	LEU	3.1
1	B	26	LEU	2.9
1	D	70	HIS	2.6
1	B	265	LEU	2.5
1	D	163	ILE	2.5
1	C	35	ASN	2.5
1	D	162	PRO	2.2
1	C	27	THR	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
3	PG4	A	278	13/13	0.71	0.23	65,70,73,73	0
3	PG4	B	277	10/13	0.74	0.20	55,60,67,67	0
3	PG4	A	279	13/13	0.80	0.22	55,66,70,71	0
3	PG4	D	278	13/13	0.81	0.19	57,63,67,68	0
3	PG4	D	277	10/13	0.84	0.15	44,52,55,56	0
3	PG4	A	277	13/13	0.85	0.18	64,68,76,76	0
2	PO4	C	276	5/5	0.97	0.06	28,32,33,34	0
2	PO4	B	276	5/5	0.98	0.07	23,26,28,28	0
2	PO4	D	276	5/5	0.98	0.05	26,26,28,30	0
2	PO4	A	276	5/5	1.00	0.03	19,20,20,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.